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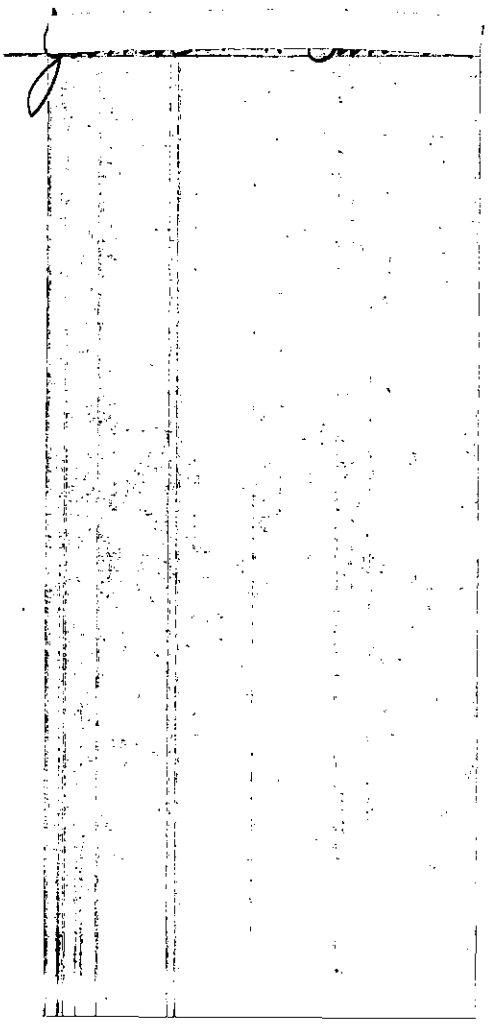

QUANTUM CELL MODEL CONSIDERATION OF THE SOLID-SUPERFLUID TRANSITION IN He^4 AT ABSOLUTE ZERO

A THESIS

Presented to

The Faculty of the Graduate Division

by

James Mervil Tanner

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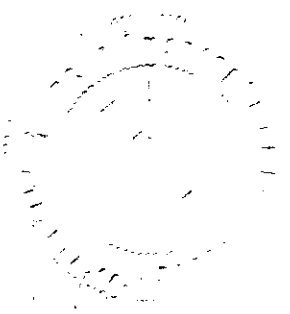

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CHAPTER I

INTRODUCTION

This investigation was undertaken as a theoretical consideration of certain experimentally observed properties of superfluid helium. In attempting to explain experimental observations on helium in its superfluid phase many investigators have, in analogy with the Bose-Einstein condensation of a gas of noninteracting bosons, tacitly assumed that the zero momentum state of the system has a macroscopic occupation. Landau (1) has attributed the superfluidity to the phonon character of the low momentum excitations in the fluid. These two concepts will be discussed in more detail later in this chapter. It is the purpose of this investigation to demonstrate that both properties are predicted by a quantum cell model for bosons.

Liquid helium under its own vapor pressure has been reduced to temperatures less than $0.1^{\circ}K$ without solidifying; this result indicates that helium can be expected to exist in the liquid state even at a temperature of absolute zero. This feature, unique to helium, is the first of a number of remarkable properties exhibited by this element at extremely low temperatures. The phase diagram for the more abundant isotope, He^4, is shown in Figure 1. The failure of the liquid to solidify under its own vapor pressure at any temperature results in the absence of a conventional triple point, i.e., the simultaneous existence of the solid, liquid, and vapor phases. He^4 exhibits two liquid

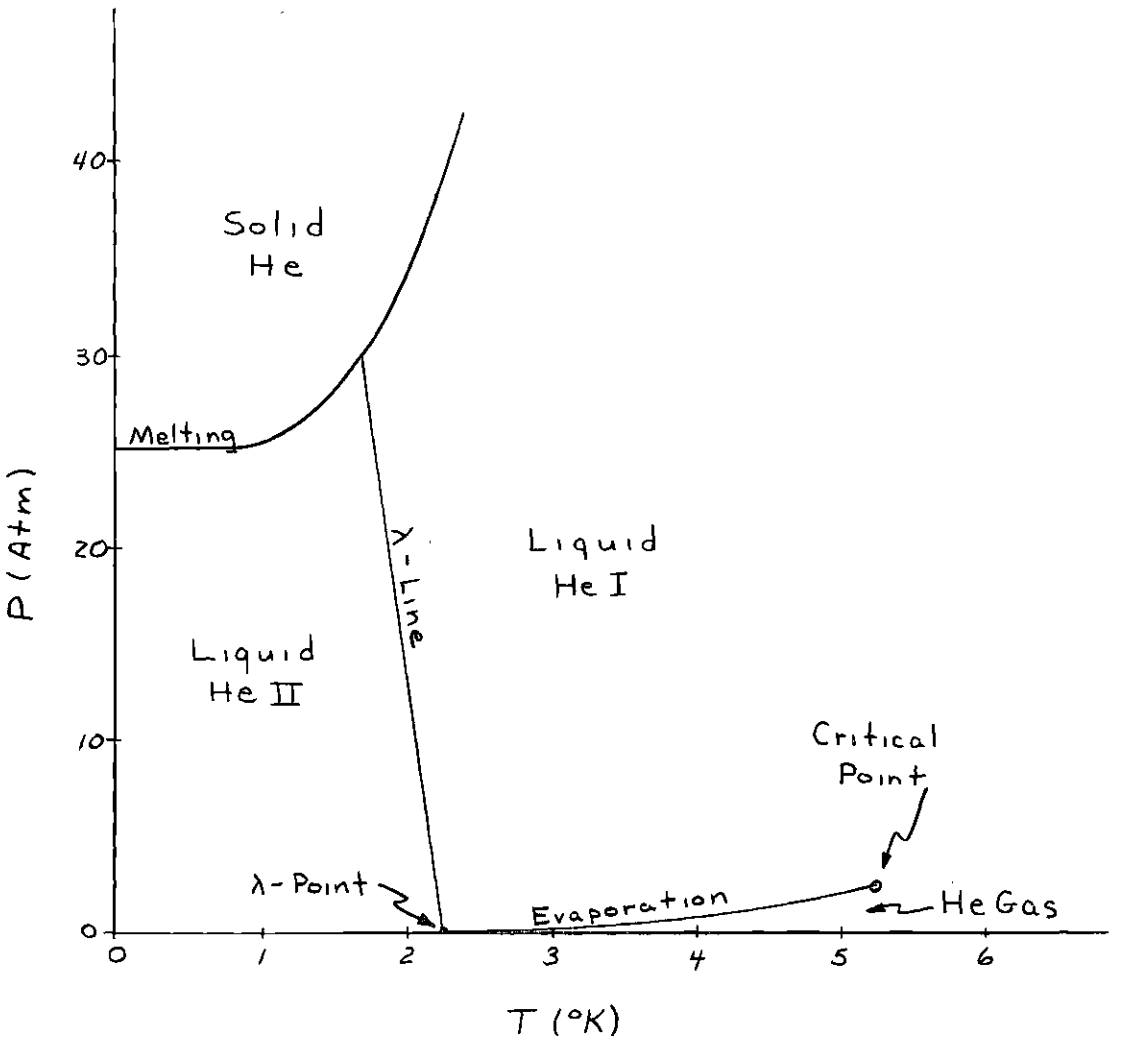

Figure 1. The Four Phases of He^4

phases, commonly denoted by He I and He II, as shown in the phase diagram. The first observation of this phase change in liquid helium was noted by Onnes (2) in 1911 when he reported that at 2.2°K liquid helium ceased contracting upon cooling and began expanding. Later measurements by Onnes and Boks displayed a discontinuous thermal expansion coefficient at 2.2°K. Specific heat measurements by Keesom and Clusius (3) exhibit a singularity in the specific heat occurring along the λ-line shown in Figure 1. The shape of this specific heat curve resembles the Greek letter λ, and the transition is therefore called the λ-transition.

The electronic structure of the helium atom consists of a pair of K-shell electrons tightly bound to a nucleus consisting of two protons and either one (He^3) or two (He^4) neutrons. The two electrons fill the K shell, and as a result helium is inactive chemically. Perhaps more important for our considerations are the extremely high ionization potential and correspondingly low electric polarizability (which is known to result in small Van der Waal's attractive forces). We see then that the helium atom is tightly bound and as a result might be expected to behave somewhat as a classical hard sphere, particularly since the attrative interaction is very small. To emphasize this point we note that helium has the highest ionization potential as well as the weakest attractive interaction of all elements.

The weak attractive forces coupled with the small mass of the helium atom offer an explanation for the reluctance of the liquid to solidify. The energy required to localize the particle to a lattice

position is approximately equal to the depth of the potential well; hence outside aid in the form of pressure is required to accomplish a change to the solid phase. The even smaller mass of hydrogen makes it likely that it might display a similar effect, but the much stronger interaction of the hydrogen atoms relative to helium dominates and thereby results in solidification for temperatures above zero. Other inert gases possess the characteristically weak interaction resulting from closed electronic shells, but their larger mass decreases the localization energy to the point where the attractive interaction still dominates. The failure of helium to solidify under its vapor pressure appears, then, to be a direct result of the nonclassical localization energy, thus prompting Landau's description of liquid helium at low temperatures as a "quantum liquid."

Since He^3 consists of an odd number of fermions with a resulting spin of 1/2, He^3 can be expected to obey Fermi-Dirac statistics while He^4, with an even number of fermions and a resulting spin of zero, submits to Bose-Einstein statistics. This subtle quantum difference apparently results in an even more striking quantum effect at low temperatures, namely, the experimental observation that He^3 does not possess the two liquid phases found in He^4. Thus the helium liquids offer a macroscopic manifestation of quantum statistics.

Since our interest in this work will be in certain properties of He^4, we shall limit our discussion to a few of its properties. While He I possesses no extraordinary properties which distinguish it from other liquids, He II exhibits a number of unique phenomena. Perhaps

the most remarkable, and certainly the best known, of these is its "superfluidity," an effect discovered simultaneously by Kapitza (4) and by Allen and Misener (5). In these experiments He II was shown to flow readily through extremely narrow capillaries with no viscosity. A second experiment using torsional oscillations of a disk immersed in He II demonstrated the same liquid to have a viscosity comparable to other liquids. Thus a paradox of some magnitude appears.

Tisza (6) offered a phenomenological solution to this paradox with his proposal of a two-fluid model. In this model He II consists of two components, a superfluid and a normal fluid. The normal fluid possesses the properties of ordinary liquids, while the superfluid has zero viscosity. Support for this two-fluid theory was found experimentally by Andronikashvili (7), who used an assembly of oscillating disks to measure the ratio of the normal component density to that of the system. This ratio is seen to decrease rapidly from unity at the λ-point to zero at $0^{\circ}K$. Atkins (8), in his comprehensive review of the experimental and theoretical status of liquid helium, asserts that the two-fluid concept is essentially correct, though possibly only a first approximation. Huang, as reported by Cohen (9), accepts the validity of the Tisza theory but points out that it is unsatisfactory primarily because it has, as yet, no molecular basis.

Theoretical treatments of liquids have been relatively unsatisfactory and have usually been accomplished by either considering the liquid as an imperfect gas in which particle interactions have become appreciable or as an imperfect solid in which local order is retained but long range order lost as a result of particle wandering.

London (10), (11), (12) pointed out the many similarities between the Bose-Einstein condensation of an ideal gas of bosons and the λ-transition of liquid helium. The ideal gas condensation corresponds to a gathering of a finite fraction of the gas particles into the lowest energy state. If one treats the particles in the lowest energy level as those forming the superfluid component and the remainder as those forming the normal component, a theoretical substantiation of Tisza's two-fluid model is obtained. Using values consistent with those of liquid helium in the Bose-Einstein condensation formalism, a transition temperature of 3.2°K is predicted in comparison with the measured value of 2.17°K. The general behavior of the specific heat of liquid helium resembles that predicted from the perfect gas.

London's characterization of the λ-transition in liquid helium as a Bose-Einstein condensation modified by the presence of interatomic forces treats the liquid as an imperfect gas and in so doing places emphasis on the wave-function of individual atoms. In contrast to this approach the theory of solids places primary consideration upon the weakly excited states resulting from the collective motion of the particles. These low energy states for the system are commonly called "elementary excitations" and can be shown to behave like particles in that they possess definite energies and momenta.

Landau (1), (13) attacked the liquid helium problem from the latter viewpoint. He suggested that the liquid at or near absolute zero consists of a system of elementary excitations in the ground state and proposed an excitation spectrum of the type shown in Figure 2.

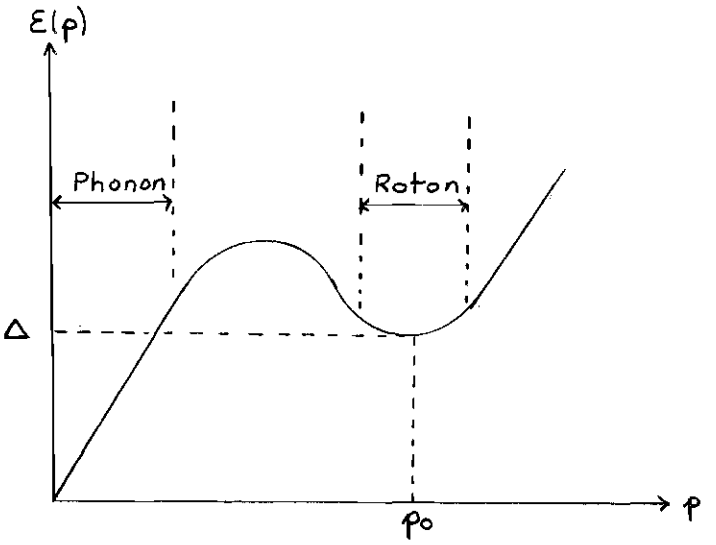

Figure 2. Excitation Spectrum for He II

This curve relates the energy $\varepsilon(p)$ of an elementary excitation to its momentum p. For small momenta the energy-momentum relationship is linear and such excitations are commonly called phonons. This type of low momentum spectrum is suggested by

(a) the knowledge from solid state that such a spectrum results in a specific heat which varies as T^3 nears absolute zero;

(b) the experimental determination of liquid helium's specific heat which exhibits a T^3 dependence in the 0°K to 0.8°K range.

In the interval between 0.8°K and the λ-point the specific heat increases more rapidly with temperature, this phenomenon indicating the presence of a second type of elementary excitation which Landau termed the roton. He selected this name since he suspected these excitations were related to the rotational nature of the liquid in contrast to the obvious translational character of the phonon. These two regions of the spectrum are

shown in Figure 2 and may be characterized by the equation

$$\varepsilon(p) = \begin{cases} cp & \text{for } p \ll p_0 \\ \Delta + \frac{(p-p_0)^2}{2\mu} & \text{for } p \sim p_0 \end{cases} . \qquad (1)$$

These excitations are assumed to obey Bose-Einstein statistics. Therefore the number with an excitation of energy $\varepsilon(p)$ at a temperature T is

$$m_p(T) = \left[e^{\frac{\varepsilon(p)}{kT}} - 1 \right]^{-1} .$$

The energy of the system at a temperature T is

$$E(T) = E_0 + \sum_p m_p(T)\,\varepsilon(p) ,$$

where E_0 is the ground state $(T = 0)$ energy; and the specific heat at constant volume is

$$C_v(T) = \left(\frac{\partial E}{\partial T}\right)_V = \sum_p \left[\frac{\partial m_p(T)}{\partial T}\right]_v \varepsilon(p) .$$

The constants c, Δ, p_0, and μ are to be adjusted for a best fit to the specific heat temperature dependence. Performing this operation Landau chose

$$c = 226 \text{ meters/sec}$$

$$\frac{\Delta}{k} = 8.9\ ^\circ\text{K}$$

$$\frac{p_0}{\hbar} = 1.99\ \text{Å}^{-1}$$

$$\mu = 0.26\, m ,$$

where k is Boltzmann's constant, $\hbar$ is Planck's constant divided by 2π, and m is the mass of the helium atom.

Cohen and Feynman (14) suggested that the excitation curve of Figure 2 could be measured by inelastic scattering of neutrons from liquid helium. These measurements were performed by Palevsky, Otnes, Larsson, Pauli, and Stedman (15) and also by Henshaw (16). Their measurements give an excitation curve in excellent agreement with Landau's proposal. For example, Henshaw reports fitted values for Δ/k and p_o/h of 8.65°K and 1.91 $\mathring{A}^{-1}$ at normal vapor pressure. These results and other successes of the Landau proposal seem to leave little doubt as to the validity of the excitation model for the liquid.

Landau (17) demonstrates that a quantum liquid with an energy spectrum as he proposes will necessarily exhibit superfluidity. This follows, as he shows, from the phonon portion of the excitation spectrum. He gives some understanding to the two-fluid theory by arguing that at absolute zero the entire system is in the quantum mechanical ground state (with no excitations) and is an ideal fluid having no viscosity. At temperatures slightly above zero, thermal energy appears in the form of elementary excitations. These excitations, possessing energy and momentum, behave as particles moving through the fluid, giving rise to the properties of an ordinary fluid, and thus account for the normal component.

Feynman (18), (19), (20) approaches the liquid helium problem by considering the Schroedinger equation for all the atoms, taking their interaction into account. Of course, a full solution is impossible,

but Feynman appears to have had some success simplifying the problem via physical intuition. He did not achieve complete success in justifying Landau's excitation spectrum in that he obtains a result for $\varepsilon(p)$ which requires a knowledge of the radial distribution function for the liquid.

A number of investigators have considered the Bose-Einstein gas with weak repulsive forces. Knollman (21) gives a brief account of these works. Application of these arguments to the superfluid problem usually incorporates the assumption that the presence of particle interactions does not remove the finite fraction of particles in the zero energy state as predicted in the Bose-Einstein condensation. Penrose and Onsager (22) consider this point in detail and conclude that a finite fraction of the particles must have identical momenta (perhaps zero but not necessarily so) at temperatures below the λ-point. They estimate that approximately eight per cent of the particles occupy this state at $0^{\circ}K$.

The approach to the superfluid from the low density region is complicated by the necessity of including attractive forces to obtain condensation of the gas and repulsive forces to insure the hard core interactions which dominate at higher densities. Basically this approach incorporates all of the as yet unsolved problems of the general gas-liquid condensation in addition to any difficulties added in obtaining the phase change in the liquid state from He I to He II. What has been done in the these works is to omit the attractive forces and confine the system with external pressure.

Some agreement with experiments on other liquids has been achieved by using lattice theories of the liquid state for classical fluids. Here the basic idea is that an average molecule in the liquid is confined to a cell formed by nearest neighbors and only occasionally moves outside this cell. Using intuitive ideas suggested by this model Gersch and Knollman (23) developed a quantum cell model for bosons. This model allows the cell size to vary with density so that the number of cells always equals the number of particles. At very high densities the particles are confined one to a cell with no fluctuations. As the density is decreased particle motion causes fluctuations. The density dependence of the model at a temperature of $0^{\circ}K$ is investigated by the use of Green's functions employed in the framework of second quantization. At high densities no condensation of a finite fraction of the particles into a single momentum state is observed. At a critical density an instability occurs in the calculation which seems to rule out extension of the results to lower densities. At this density, however, the excitation spectrum as calculated from the Green's functions changes from quadratic to linear for small momenta.

It is the purpose of this work to investigate carefully the approximations used to get the results by Gersch and Knollman, to consider the solutions for the Green's functions in some detail, and to attempt to obtain solutions for densities less than the critical density. Chapter II reviews the formulation of the cell model and points out a few features of the model in the high density limit. Green's functions for the cell model are defined in Chapter III, their characteristics are

studied in some detail, and differential equations of motion for their time dependence are obtained. These equations of motion constitute a set of coupled differential equations which are apparently intractable. Thus it becomes necessary to make approximations consistent with the nature of the cell model in the high density region. Chapter IV deals with these approximations. A discussion of the solution of the equations of motion and the final approximations needed for a solution are the subject of Chapter V. The solution of the resulting equations of motion is obtained in Chapter VI. A procedure is found for extending the solutions into the superfluid region while simultaneously retaining the phonon portion of the excitation spectrum. It is also shown that whereas no momentum state possesses finite occupation for densities greater than the critical density, for densities less than this critical value a finite fraction is observed in the zero momentum state.

CHAPTER II

THE CELL MODEL HAMILTONIAN

Consider a system of spinless, nonrelativistic bosons which interact pairwise according to the potential $U(r)$, where r is the separation between the two particles. The Hamiltonian operator for such a system is

$$H = \tfrac{1}{2}\int \Psi^{+}(r)\,\Psi^{+}(r')\,U(r-r')\,\Psi(r')\,\Psi(r)\,d\tau'd\tau + \frac{\hbar^2}{2m}\int \nabla\Psi^{+}(r)\cdot\nabla\Psi(r)\,d\tau ,$$

where the field operators $\psi^{+}(r)$ and $\psi(r)$ obey the commutation relations

$$\left[\Psi(r),\ \Psi^{+}(r')\right] = \delta(r-r') \tag{2}$$

$$\left[\Psi(r),\ \Psi(r')\right] = \left[\Psi^{+}(r),\ \Psi^{+}(r')\right] = 0 .$$

The particle-number operator for such a system is

$$N = \int \Psi^{+}(r)\,\Psi(r)\,d\tau ,$$

while the linear momentum operator is defined by

$$P = -\frac{i\hbar}{2}\int\left\{\Psi^{+}(r)\left[\nabla\Psi(r)\right] - \left[\nabla\Psi^{+}(r)\right]\Psi(r)\right\}d\tau . \tag{3}$$

We now introduce a spatial extent $(2L)^3$ by imposing the following boundary conditions on the field operators:

$$\Psi(x_1+2L,\,x_2,\,x_3) = \Psi(x_1,\,x_2+2L,\,x_3) = \Psi(x_1,\,x_2,\,x_3+2L) = \Psi(x_1,x_2,x_3) .$$

With this periodicity $\psi(r)$ may be expanded in terms of a new operator, α_k, by the Fourier series

$$\Psi(r) = (2L)^{-3/2} \sum_{k_x=-\infty}^{\infty} \alpha_k \, e^{\frac{2\pi i k \cdot r}{2L}} , \tag{4}$$

where k is a vector with three components, each of which is an integer. Inverting the series expansion to obtain an explicit expression for the operator α_k yields

$$\alpha_k = (2L)^{-3/2} \int_R \Psi(r) \, e^{-\frac{2\pi i k \cdot r}{2L}} \, d\tau , \tag{5}$$

where R is the volume defined by

$$-L \leq x_1, x_2, x_3 \leq L .$$

The α_k^+ and α_k operators satisfy the commutation relations

$$\left[\alpha_k , \alpha_{k'}^+\right] = \delta_{k,k'}$$

$$\left[\alpha_k , \alpha_{k'}\right] = \left[\alpha_k^+ , \alpha_{k'}^+\right] = 0 ,$$

which follow directly from Equations (2) and (5). They are to be interpreted as creation and destruction operators, respectively, for particles of momentum $hk/2L$, as we shall see. Expansion of the linear momentum operator in terms of these operators by substituting for $\psi^+(r)$ and $\psi(r)$ from Equation (4) into Equation (3) gives

$$P = -\frac{ih}{2} \frac{1}{(2L)^3} \sum_{k k'} \alpha_k^+ \alpha_{k'} \left(\frac{2\pi i}{2L}\right)(k+k') \int_R e^{\frac{2\pi i (k-k')\cdot r}{2L}} \, d\tau .$$

Now

$$\int_R e^{\frac{2\pi i (k-k')\cdot r}{2L}} \, d\tau = (2L)^3 \, \delta_{k,k'} ,$$

so that

$$P = \sum_k \frac{h k}{2L} \alpha_k^+ \alpha_k \quad .$$

The kinetic energy operator may be expressed in terms of the momentum operator as follows:

$$T = \frac{\hbar^2}{2m} \int_R \nabla \psi^+(r) \cdot \nabla \psi(r) \, d\tau$$

$$= \frac{\hbar^2}{2m} \frac{1}{(2L)^3} \sum_{kk'} \left(-\frac{2\pi i}{2L}\right)\left(\frac{2\pi i}{2L}\right) k \cdot k' \, \alpha_k^+ \alpha_{k'} \int_R e^{\frac{2\pi i (k'-k)\cdot r}{2L}} d\tau$$

$$= \sum_k \frac{1}{2m} \left(\frac{h k}{2L}\right)^2 \alpha_k^+ \alpha_k \quad .$$

Similarly the number operator becomes

$$N = \int_R \psi^+(r) \psi(r) \, d\tau = \frac{1}{(2L)^3} \sum_{kk'} \alpha_k^+ \alpha_{k'} \int_R e^{\frac{2\pi i (k'-k)\cdot r}{2L}} d\tau$$

$$= \sum_k \alpha_k^+ \alpha_k \quad .$$

Similar operations to express the potential energy operators in terms of the momentum operators give

$$V = \frac{1}{2} \int_R \psi^+(r) \, \psi^+(r') \, U(r-r') \, \psi(r') \, \psi(r) \, d\tau' d\tau$$

$$= \frac{1}{2} \sum_{k_1} \sum_{k_2} \sum_{k_3} \sum_{k_4} \alpha_{k_1}^+ \alpha_{k_2}^+ \alpha_{k_3} \alpha_{k_4} \, g(k_1, k_2, k_3, k_4) \quad ,$$

where

$$g(k_1, k_2, k_3, k_4) = \frac{1}{(2L)^3} \int_R e^{\frac{2\pi i (k_4 - k_1)\cdot r}{2L}} U(r-r') \, e^{\frac{2\pi i (k_3 - k_2)\cdot r'}{2L}} d\tau' \, d\tau$$

In this expression for g let us make the change of variables

$$r'' = r - r' \qquad\qquad r = r$$

so that

$$g(k_1,k_2,k_3,k_4) = \frac{1}{(2L)^3}\int_R e^{\frac{2\pi i(k_4+k_3-k_2-k_1)\cdot r}{2L}}\left\{\int_{R^*} U(r'')\, e^{\frac{2\pi i(k_3-k_2)\cdot r''}{2L}} d\tau''\right\} d\tau .$$

Now the region, R^*, over which the r'' integral is to be evaluated depends upon r and thus g cannot, in general, be written as the product of two definite integrals. If we assume $U(r)$ to have a range D, such that $D << L$, then the r'' integral may be approximated very accurately by

$$\int_{r''\le D} U(r'')\, e^{\frac{2\pi i(k_3-k_2)\cdot r''}{2L}} d\tau'' .$$

The error in such an approximation occurs when the vector r is within a distance D of the boundary of R. Thus, if we confine our considerations to systems whose linear dimensions are large compared to the interaction range, then

$$g(k_1,k_2,k_3,k_4) = U(k_3-k_2)\,\delta_{k_1+k_2,k_3+k_4} ,$$

where

$$U(k_3-k_2) = \frac{1}{(2L)^3}\int_{r''\le D} U(r'')\, e^{\frac{2\pi i(k_3-k_2)\cdot r''}{2L}} d\tau'' .$$

The resulting expression for the potential energy operator is then

$$V = \frac{1}{2}\sum_{k_1}\sum_{k_2}\sum_{k_3} U(k_3-k_2)\,\alpha^+_{k_1}\alpha^+_{k_2}\alpha_{k_3}\alpha_{k_1+k_2-k_3} .$$

Since the operators H, T, and V are invariant under an infinitesimal coordinate translation, and since the linear momentum operator is the generator of such a translation, we expect that P should commute with each of the energy operators. Now

$$[P, V] = \frac{h}{4L}\sum_{k}\sum_{k_1}\sum_{k_2}\sum_{k_3} k\, U(k_3-k_2)\left[\alpha^+_k\alpha_k\,,\ \alpha^+_{k_1}\alpha^+_{k_2}\alpha_{k_3}\alpha_{k_1+k_2-k_3}\right] .$$

and

$$\left[\alpha_k^+\alpha_k,\ \alpha_{k_1}^+\alpha_{k_2}^+\alpha_{k_3}\alpha_{k_1+k_2-k_3}\right] = \alpha_{k_1}^+\alpha_{k_2}^+\alpha_{k_3}\alpha_{k_1+k_2-k_3}\left[\delta_{k,k_1}+\delta_{k,k_2}-\delta_{k,k_3}-\delta_{k,k_1+k_2-k_3}\right].$$

Hence

$$[P,V] = \frac{h}{4L}\sum_{k_1}\sum_{k_2}\sum_{k_3}\alpha_{k_1}^+\alpha_{k_2}^+\alpha_{k_3}\alpha_{k_1+k_2-k_3}\sum_k k\left[\delta_{k,k_1}+\delta_{k,k_2}-\delta_{k,k_3}-\delta_{k,k_1+k_2-k_3}\right] = 0.$$

Similarly

$$[P,T] = \frac{1}{2m}\left(\frac{h}{2L}\right)^3\sum_k\sum_{k'}(k\cdot k)\,k'\left[\alpha_{k'}^+\alpha_{k'},\ \alpha_k^+\alpha_k\right];$$

but

$$\left[\alpha_{k'}^+\alpha_{k'},\ \alpha_k^+\alpha_k\right] = 0,$$

so that

$$[P,T] = 0.$$

It follows that

$$[P,H] = [P,\ T+V] = [P,T] + [P,V] = 0.$$

That the potential and kinetic energy operators do not commute is shown in the following:

$$\begin{aligned}[T,V] &= \frac{1}{4m}\left(\frac{h}{2L}\right)^2\sum_k\sum_{k_1}\sum_{k_2}\sum_{k_3}k^2\,U(k_3-k_2)\left[\alpha_k^+\alpha_k,\ \alpha_{k_1}^+\alpha_{k_2}\alpha_{k_3}\alpha_{k_1+k_2-k_3}\right]\\ &= \frac{1}{4m}\left(\frac{h}{2L}\right)^2\sum_{k_1}\sum_{k_2}\sum_{k_3}U(k_3-k_2)\,\alpha_{k_1}^+\alpha_{k_2}^+\alpha_{k_3}\alpha_{k_1+k_2-k_3}\sum_k k^2\left[\delta_{k,k_1}+\delta_{k,k_2}-\delta_{k,k_3}-\delta_{k,k_1+k_2-k_3}\right]\\ &= \frac{1}{2m}\left(\frac{h}{2L}\right)^2\sum_{k_1}\sum_{k_2}\sum_{k_3}U(k_3-k_2)\,(k_1-k_3)\cdot(k_2-k_3)\,\alpha_{k_1}^+\alpha_{k_2}^+\alpha_{k_3}\alpha_{k_1+k_2-k_3}\\ &\neq 0.\end{aligned}$$

Therefore

$$[T, H] = [T, T+V] = [T, T] + [T, V] = [T, V] \neq 0,$$

and

$$[V, H] = [V, T+V] = [V, T] + [V, V] = [V, T] \neq 0.$$

We conclude that eigenstates of any one of the operators H, T, and V cannot be eigenstates of either of the remaining two, while eigenstates of either H, T, or V may be selected such that they are also eigenstates of P.

Cell Space and Cell Operators

Let us now partition the region R into $N_0 = (2N + 1)^3$ equal subregions (or cells) of volume $(2a)^3$ where

$$a = \frac{L}{2N+1} \quad ,$$

with the midpoint of the cells being located by

$$r_\ell = 2a\ell \, ,$$

where ℓ is a 3-component vector given by

$$\ell = \ell_1 e_1 + \ell_2 e_2 + \ell_3 e_3 \, , \qquad \ell_i = 0, \pm 1, \pm 2, \cdots, \pm N.$$

e_1, e_2, and e_3 are unit vectors in the directions x_1 x_2, x_3, respectively.

The cell model operators are obtained by the following procedure:

For r within cel ℓ the field operator is replaced by its average over this cell, i.e.,

$$\Psi(r) \longrightarrow \rho \int_{\ell} \Psi(r)\, d\tau \ ,$$

where $\rho = (2a)^{-3}$ is the number of cells per unit volume. Now define the cell operator b_{ℓ} by

$$b_{\ell} = \rho^{1/2} \int_{\ell} \Psi(r)\, d\tau \ ,$$

so that

$$\Psi(r) = \rho^{1/2} b_{\ell} \qquad \text{for } r \text{ in cell } \ell.$$

If we define the function

$$\delta_{r,\ell} = \left\{ \begin{array}{ll} 1 & \text{for } r \text{ in } \ell \\ 0 & \text{otherwise} \end{array} \right\} \ ,$$

then the cell model operator replacing the field operator is

$$\Psi(r) \longrightarrow \rho^{1/2} \sum_{\ell} b_{\ell}\, \delta_{r,\ell} \ .$$

Let us also define a cell model approximation to the pair interaction potential, namely

$$U(r-r') \longrightarrow \sum_{\ell} \rho U_0(\rho)\, \delta_{r,\ell}\, \delta_{r',\ell} + \sum_{\ell \neq \ell'} \sum U_{\ell,\ell'}(\rho)\, \delta_{r,\ell}\, \delta_{r',\ell'} \ .$$

Thus two particles in the same cell possess an interaction energy $\rho U_0(\rho)$, while the two particles when occupying different cells, say ℓ_1 and ℓ_2, interact with an energy $U_{\ell_1 \ell_2}(\rho)$. Notice that the interaction energy, in any case, is determined by the cell locations of the pair and is independent of the particles' positions within the confines of the cell. The cell interaction is permitted to vary with the cell

size as denoted in the ρ-dependence. Hence the $U(\rho)$ functions are, in essence, functions which may be chosen in an effort to most nearly approximate the correct interaction.

We turn our attention now to obtaining cell operators for the potential and kinetic energy operators. Using Equations (7) and (8) in the expression for the potential energy operator, we get

$$V = \tfrac{1}{2}\iint \Psi^+(r)\,\Psi^+(r')\,U(r-r')\,\Psi(r')\,\Psi(r)\,d\tau'\,d\tau$$

$$\rightarrow \tfrac{1}{2}\rho^2 \sum_{\ell_1}\sum_{\ell_2}\sum_{\ell_3}\sum_{\ell_4} b^+_{\ell_1} b^+_{\ell_2} b_{\ell_3} b_{\ell_4} \iint \left[\delta_{r,\ell_1}\delta_{r';\ell_2}\delta_{r';\ell_3}\delta_{r,\ell_4}\right] \cdot \left[\sum_{\ell}\rho U_0\,\delta_{r,\ell}\delta_{r';\ell} + \sum_{\ell\neq\ell'}\sum U_{\ell,\ell'}\,\delta_{r,\ell}\delta_{r';\ell'}\right] d\tau'\,d\tau$$

$$= \left\{ \begin{array}{l} \tfrac{1}{2}\rho^2 \sum_{\ell_1}\sum_{\ell_2}\sum_{\ell_3}\sum_{\ell_4}\sum_{\ell} b^+_{\ell_1} b^+_{\ell_2} b_{\ell_3} b_{\ell_4}\,\rho U_0 \iint \delta_{r,\ell_1}\delta_{r';\ell_2}\delta_{r';\ell_3}\delta_{r,\ell_4}\delta_{r,\ell}\delta_{r';\ell}\,d\tau'\,d\tau \\ + \tfrac{1}{2}\rho^2 \sum_{\ell_1}\sum_{\ell_2}\sum_{\ell_3}\sum_{\ell_4}\sum_{\ell\neq\ell'} b^+_{\ell} b^+_{\ell_2} b_{\ell_3} b_{\ell_4}\,U_{\ell,\ell'} \iint \delta_{r,\ell_1}\delta_{r';\ell_2}\delta_{r';\ell_3}\delta_{r,\ell_4}\delta_{r,\ell}\delta_{r';\ell'}\,d\tau'\,d\tau \end{array} \right\}$$

$$= \left\{ \begin{array}{l} \tfrac{1}{2}\rho^2 \sum_{\ell_1}\sum_{\ell_2}\sum_{\ell_3}\sum_{\ell_4}\sum_{\ell} \rho U_0\, b^+_{\ell_1} b^+_{\ell_2} b_{\ell_3} b_{\ell_4}\,\delta_{\ell_1,\ell}\delta_{\ell_2,\ell}\delta_{\ell_3,\ell}\delta_{\ell_4,\ell} \int_{\ell} d\tau' \int_{\ell} d\tau \\ + \tfrac{1}{2}\rho^2 \sum_{\ell_1}\sum_{\ell_2}\sum_{\ell_3}\sum_{\ell_4}\sum_{\ell\neq\ell'} U_{\ell,\ell'}\, b^+_{\ell_1} b^+_{\ell_2} b_{\ell_3} b_{\ell_4}\,\delta_{\ell_1,\ell}\delta_{\ell_2,\ell'}\delta_{\ell_3,\ell'}\delta_{\ell_4,\ell} \int_{\ell'} d\tau' \int_{\ell} d\tau \end{array} \right\}$$

$$= \tfrac{1}{2}\rho\,U_0(\rho)\sum_{\ell} b^+_{\ell} b^+_{\ell} b_{\ell} b_{\ell} + \tfrac{1}{2}\sum_{\ell\neq\ell'}\sum U_{\ell,\ell'}(\rho)\, b^+_{\ell} b^+_{\ell'} b_{\ell'} b_{\ell} \,. \qquad (9)$$

To interpret this result let us investigate the cell operators, b_ℓ and b^+_ℓ, in some more detail. Recall that the field operator, $\psi(r)$, is an operator which annihilates a particle at r. Since b_ℓ is defined by Equation (6), we are led to interpret this operator as one which annihilates a particle within the cell ℓ. Similarly b^+_ℓ is to be associated with the creation of a particle within cell ℓ.

The commutation relations governing these operators are obtained by use of the corresponding relations for the field operators. For instance

$$[b_\ell, b_{\ell'}^+] = \rho \int_\ell d\tau \int_{\ell'} d\tau' \, [\psi(r), \psi^+(r')]$$

$$= \rho \int_\ell d\tau \int_{\ell'} d\tau' \, \delta(r-r')$$

$$= \rho \int_\ell d\tau \; \delta_{\ell,\ell'}$$

or

$$[b_\ell, b_{\ell'}^+] = \delta_{\ell,\ell'} \; . \tag{10}$$

Similarly

$$[b_\ell, b_{\ell'}] = \rho \int_\ell d\tau \int_{\ell'} d\tau' \, [\psi(r), \psi(r')] = 0 \tag{11}$$

$$[b_\ell^+, b_{\ell'}^+] = \rho \int_\ell d\tau \int_{\ell'} d\tau' \, [\psi^+(r), \psi^+(r')] = 0 \; . \tag{12}$$

Now the number operator for cell ℓ is

$$n_\ell = \int_\ell \psi^+(r) \, \psi(r) \, d\tau \; ,$$

which in the cell approximation becomes

$$n_\ell \longrightarrow \rho \int_\ell b_\ell^+ b_\ell \, d\tau = b_\ell^+ b_\ell \, \rho \int_\ell d\tau$$

or

$$n_\ell = b_\ell^+ b_\ell \; . \tag{13}$$

That n_ℓ is an operator with eigenvalues 0, 1, 2, ... follows immediately from the commutation relations for the operators b_ℓ^+ and b_ℓ.

Using Equations (10), (11), (12), and (13) in Equation (9) we see that the potential energy operator may be written

$$V = \tfrac{1}{2}\rho U_0 \sum_{\ell} m_\ell (m_\ell - 1) + \tfrac{1}{2} \sum_{\ell \neq \ell'} \sum U_{\ell,\ell'} m_\ell m_{\ell'} \ . \qquad (14)$$

Thus, singly-occupied cells contribute to the potential energy only by interaction with other occupied cells through the interaction energy $U_{\ell,\ell'}$, while cells with two or more particles contribute, in addition, an integral multiple of ρU_0.

The kinetic energy operator for the continuum is

$$T = \frac{\hbar^2}{2m} \int \nabla \psi^+(r) \cdot \nabla \psi(r)\, d\tau = \frac{\hbar^2}{2m} \sum_{i=1}^{3} \int \frac{\partial \psi^+(r)}{\partial x_i} \frac{\partial \psi(r)}{\partial x_i}\, d\tau \ .$$

To obtain a cell model representation for this operator requires a cell model equivalent to the differentiation process since T involves terms like $\partial\psi/\partial x_1$. Heretofore $\psi(r)$ has been assigned a constant value within a cell. For the cell model approximation to $\partial\psi/\partial x_1$ we use a difference formula, namely

$$\frac{\partial \psi(x_1, x_2, x_3)}{\partial x_1} \longrightarrow \frac{\psi(x_1 + 2a, x_2, x_3) - \psi(x_1, x_2, x_3)}{2a} \ .$$

Now for r in cell ℓ (and hence $r + 2ae_1$ in cell $\ell + e_1$),

$$\psi(x_1 + 2a, x_2, x_3) \longrightarrow \rho^{1/2} b_{\ell + e_1}$$

$$\psi(x_1, x_2, x_3) \longrightarrow \rho^{1/2} b_\ell \ ,$$

so that

$$\frac{\partial \psi(r)}{\partial x_1} \longrightarrow \frac{\rho^{1/2}}{2a} (b_{\ell + e_1} - b_\ell) \ .$$

Similarly

$$\frac{\partial \psi^+(r)}{\partial x_1} \longrightarrow \frac{\rho^{1/2}}{2a} (b^+_{\ell + e_1} - b^+_\ell) \ ;$$

and for arbitrary r,

$$\frac{\partial \psi(r)}{\partial x_1} \longrightarrow \frac{\rho^{1/2}}{2a} \sum_{\ell} (b_{\ell+e_1} - b_\ell)\, \delta_{r,\ell}$$

$$\frac{\partial \psi^+(r)}{\partial x_1} \longrightarrow \frac{\rho^{1/2}}{2a} \sum_{\ell} (b^+_{\ell+e_1} - b^+_\ell)\, \delta_{r,\ell} \,.$$

Therefore we have

$$\frac{\partial \psi^+(r)}{\partial x_1} \frac{\partial \psi(r)}{\partial x_1} \longrightarrow \frac{\rho}{(2a)^2} \sum_{\ell} \sum_{\ell'} (b^+_{\ell+e_1} - b^+_\ell)(b_{\ell'+e_1} - b_{\ell'})\, \delta_{r,\ell}\, \delta_{r,\ell'} \,.$$

Integrating over $-L \le x_i \le L$, we get

$$\int \frac{\partial \psi^+(r)}{\partial x_1} \frac{\partial \psi(r)}{\partial x_1} d\tau \longrightarrow \frac{\rho}{(2a)^2} \sum_{\ell} \sum_{\ell'} (b^+_{\ell+e_1} - b^+_\ell)(b_{\ell'+e_1} - b_{\ell'}) \int \delta_{r,\ell}\, \delta_{r,\ell'}\, d\tau \,.$$

Now

$$\int \delta_{r,\ell}\, \delta_{r,\ell'}\, d\tau = \delta_{\ell,\ell'} \int d\tau = \delta_{\ell,\ell'} (2a)^3 = \rho^{-1} \delta_{\ell,\ell'} \,,$$

so that

$$\begin{aligned} \int \frac{\partial \psi^+(r)}{\partial x_1} \frac{\partial \psi(r)}{\partial x_1} d\tau \longrightarrow & \frac{1}{(2a)^2} \sum_{\ell} (b^+_{\ell+e_1} - b^+_\ell)(b_{\ell+e_1} - b_\ell) \\ &= \frac{1}{(2a)^2} \sum_{\ell} (b^+_{\ell+e_1} b_{\ell+e_1} + b^+_\ell b_\ell - b^+_{\ell+e_1} b_\ell - b^+_\ell b_{\ell+e_1}) \\ &= \rho^{2/3} \sum_{\ell} (2 b^+_\ell b_\ell - b^+_\ell b_{\ell+e_1} - b^+_\ell b_{\ell-e_1}) \,. \end{aligned}$$

The cell model kinetic energy operator is now

$$T \longrightarrow \frac{\hbar^2 \rho^{2/3}}{2m} \left[6 \sum_{\ell} b^+_\ell b_\ell - \sum_{\ell} \sum_{r'} b^+_\ell b_{\ell+r'} \right]. \qquad (15)$$

where the r' sum is simply

$$\sum_{r'} b_{\ell}^{+} b_{\ell+r'} = \sum_{i=1}^{3} \left(b_{\ell}^{+} b_{\ell+e_i} + b_{\ell}^{+} b_{\ell-e_i} \right).$$

The constant multiplying the two sums of Equation (15) represents the energy required to localize a particle within a cell of volume $(2a)^3$. Let us define the constant K by

$$K = \frac{\hbar^2 \rho^{2/3}}{2m} ,$$

so that

$$T \longrightarrow 6K \sum_{\ell} m_{\ell} - K \sum_{\ell} \sum_{r'} b_{\ell}^{+} b_{\ell+r'} . \tag{16}$$

From Equations (14) and (16) we obtain the cell model Hamiltonian operator

$$H = \tfrac{1}{2} \rho U_0 \sum_{\ell} m_{\ell}(m_{\ell}-1) + \tfrac{1}{2} \sum_{\ell \neq \ell'} \sum U_{\ell,\ell'} m_{\ell} m_{\ell'} + 6K \sum_{\ell} m_{\ell} - K \sum_{\ell} \sum_{r'} b_{\ell}^{+} b_{\ell+r'} . \tag{17}$$

For this work the Hamiltonian will be simplified by neglect of the contribution to the potential energy by particles in different cells, i.e., we set $U_{\ell,\ell'} \equiv 0$. While this decreases the accuracy with which any pair interaction may be represented, it effects a major simplification in the calculation to follow. For cell sizes comparable to, or larger than, the interaction range, the $U_{\ell,\ell'}$ terms should be small compared to ρU_0. Thus the Hamiltonian to be treated here is

$$H = \tfrac{1}{2} \rho U_0 \sum_{\ell} m_{\ell}(m_{\ell}-1) + 6K \sum_{\ell} m_{\ell} - K \sum_{\ell} \sum_{r'} b_{\ell}^{+} b_{\ell+r'} . \tag{18}$$

Let us rewrite the Hamiltonian of Equation (18) in the form

$$H = \tfrac{1}{2} \rho U_0 \left[\sum_{\ell} m_{\ell}(m_{\ell}-1) + 6x \sum_{\ell} m_{\ell} - x \sum_{\ell} \sum_{r'} b_{\ell}^{+} b_{\ell+r'} \right] ,$$

where the parameter x, defined by

$$x = \frac{2K}{\rho U_0} = \frac{2\hbar^2 \rho^{2/3}}{2m} \frac{1}{\rho U_0} = \frac{\hbar^2}{m \rho^{1/3} U_0} ,$$

measures the ratio of the kinetic energy of localization within the cell to the potential energy of interaction between two particles within the same cell. For sufficiently high densities ρU_0 should increase at least as fast as ρ to reflect the hard core interaction between particles. Thus for sufficiently high densities x must go to zero faster than $\rho^{-1/3}$. We conclude then that the high density characteristics of the cell model are dominated by the potential energy term, i.e.,

$$H(\rho \to \infty) \longrightarrow V = \tfrac{1}{2} \rho U_0 \sum_\ell n_\ell (n_\ell - 1) .$$

Let $|\psi\rangle$ be an arbitrary state. The expectation value for V is then

$$\langle V \rangle = \langle \Psi | V | \Psi \rangle = \tfrac{1}{2} \rho U_0 \sum_\ell \langle \Psi | n_\ell (n_\ell - 1) | \Psi \rangle .$$

Since $|\psi\rangle$ may be expanded in states diagonalized in occupation number space, and since $\langle n_\ell (n_\ell - 1) \rangle$ for such a state is $1 \cdot 0$, $2 \cdot 1$, $3 \cdot 2$, ... only, we concluded that $\langle \psi | n_\ell (n_\ell - 1) | \psi \rangle \geq 0$ and therefore

$$\langle \Psi | V | \Psi \rangle \geq 0 . \tag{19}$$

Since V is diagonal in n_ℓ, any state diagonal in occupation number space must be an eigenstate of V. For instance, consider the completely localized state with one particle per cell denoted by $|n_j - 1\rangle$. Now

$$V|m_j=1\rangle = \tfrac{1}{2}\rho U_0 \sum_\ell m_\ell(m_\ell-1)\,|m_j=1\rangle = 0.$$

Thus this localized state is an eigenstate of the potential energy operator corresponding to a potential energy of zero.

Let N_0 be the total number of cells, i.e.,

$$N_0 = (2N+1)^3.$$

Consider any N_0-particle state in occupation-number space. If this space differs from the localized state, it must differ by the presence of some cells with zero occupancy and some with multiple occupancy. For instance consider the state with a zero occupancy in cell ℓ_1 and a double occupancy in cell ℓ_2, denoted by $|n_j - 1 + \delta_{j\ell_2} - \delta_{j\ell_1}\rangle$. Now

$$V|m_j=1+\delta_{j\ell_2}-\delta_{j\ell_1}\rangle = \tfrac{1}{2}\rho U_0 \sum_\ell m_\ell(m_\ell-1)\,|m_j=1+\delta_{j\ell_2}-\delta_{j\ell_1}\rangle$$

$$= \rho U_0\,|m_j=1+\delta_{j\ell_2}-\delta_{j\ell_1}\rangle.$$

Thus this state is an eigenstate of V corresponding to the eigenvalue ρU_0. We see then, that any change from the localized state necessitates the creation of at least one multiply-occupied cell and results in an eigenvalue for $V > 0$. Since any eigenvalue of V must be greater than or equal to zero by Equation (19), and since the localized state is the only N_0-particle state yielding an eigenvalue of zero, we conclude that the localized state constitutes the ground state of the system for sufficiently high densities. It follows immediately that the high-density ground state for $N_0 - 1$ particles has one zero occupancy and $N_0 - 1$ single occupancies with a V-eigenvalue of 0. Similarly the $(N_0 + 1)$-

particle ground state has one double occupancy and $N_o - 1$ single occupancies with a V-eigenvalue of ρU_o.

If we, for the moment, neglect the kinetic energy contribution, we conclude that the energy (μ^-) required to add a particle to the $(N_o - 1)$-particle ground state and create the N_o-particle ground state is zero, while the energy (μ^+) required to add a particle to the N_o-particle ground state and create the $(N_o + 1)$-particle ground state is ρU_o, i.e.,

$$\mu^- = 0$$

$$\mu^+ = \rho U_o .$$

The symbol μ is used here since this quantity would seem to be the $T = 0$ extension of the chemical potential, defined by

$$\mu = \left(\frac{\partial E}{\partial N}\right)_{S,V} .$$

The argument presented thus far has assumed that the cell model Hamiltonian is completely dominated at very high densities by the potential energy term. As a result, it is demonstrated that the ground state is a completely localized state. All kinetic energy contributions have been neglected, and as a result the N_o-particle ground state has a zero energy. This localized state is also an eigenstate of the diagonal part of the kinetic energy, namely $6K \sum_{\ell} n_\ell$, with an eigenvalue $6KN_o$. If we wish to include this portion of the kinetic energy in the energy operator, it does not affect the previous arguments as to the nature of the high-density ground state since any N_o-particle state corresponds

to an eigenvalue of $6KN_o$, and thus shifts all states up by $6KN_o$. In such a case, our modified Hamiltonian is

$$H = \tfrac{1}{2} \rho U_o \sum_\ell m_\ell (m_\ell - 1) + 6K \sum_\ell m_\ell ,$$

and the corresponding ground state energies for the $(N_o - 1)$-, N_o-, and $(N_o + 1)$-particle states are

$$E_o(N_o-1) = 6K(N_o-1)$$

$$E_o(N_o) = 6K N_o$$

$$E_o(N_o+1) = \rho U_o + 6K(N_o+1),$$

so that the chemical potentials defined earlier are

$$\mu^- = E_o(N_o) - E_o(N_o-1) = 6K$$

$$\mu^+ = E_o(N_o+1) - E_o(N_o) = \rho U_o + 6K .$$

The second term in the kinetic energy operator, namely, $-K \sum_\ell \sum_{r'} b_\ell^+ b_{\ell+r'}$, causes a lowering of the kinetic energy by delocalization of the particles. It is this term which makes the Hamiltonian nondiagonal in occupation number space. The ground state of the full Hamiltonian will, as a result, consist of a superposition of the occupation number states. The potential energy thus tends to localize the particles while this nondiagonal kinetic energy term causes multiply-occupied cells. At very high densities the lowering effect by the kinetic energy is vanishingly small compared to the increase (ρU_o) in the potential energy resulting from just one doubly-occupied cell. This localization of particles, one to a cell, at high densities we interpret

as the cell model representation of the solid. As the density decreases the particles will exhibit increasing wanderings. This delocalization effect should be reflected in increased values for fluctuation parameters such as $\langle n(n-1)\rangle$ which vanishes for the localized state. The solid characteristics seen for high densities can be expected, therefore, to "wash out" as the density decreases. We shall demonstrate that as this effect occurs μ^- and μ^+ approach one another in value, and for a particular value of $x > 0$ (and hence ρ) the two coalesce. It is at this point that the solid-like nature disappears and a transition of some type is suggested.

It should be noted that the Hamiltonian of Equation (17) was developed by Gersch and Knollman (23). In their work they demonstrate (a) that the Hamiltonian yields the correct energy-momentum relationship for free particles $(U_o = 0)$ with low momentum, and (b) that for low densities such that $\rho U_o << K$, the Hamiltonian yields the correct expression for the energy of low-momentum excitations.

CHAPTER III

GREEN'S FUNCTIONS FOR THE CELL MODEL

In Chapter I two questions related to the superfluid problem were proposed. First, can one obtain Landau's elementary excitation curve by starting from a system Hamiltonian including interparticle forces? Second, can one verify that a macroscopic occupation of the zero momentum state occurs in the superfluid phase? The model to be used in considering these questions is the cell Hamiltonian developed in Chapter II, and the analytical technique to be employed is the Green's function formalism. This formalism is chosen since, as we shall demonstrate in this and subsequent chapters, Green's functions provide direct access to answers for the two questions listed above.

In this chapter we define a hierarchy of double-time Green's functions for the cell model, study analytical properties of these Green's functions, and obtain differential equations of motion for the members of this set.

Before defining the Green's functions a few additional comments on the Hamiltonian and its properties are needed. Since the Hamiltonian

$$H = \tfrac{1}{2} \rho U_0 \sum_{\ell} m_\ell (m_\ell - 1) + 6K \sum_{\ell} m_\ell - K \sum_{\ell} \sum_{r=1} b_\ell^+ b_{\ell+r} ,$$

does not alter the number of particles in any state upon which it acts, it commutes with the number operator

$$N = \sum_{\ell} m_\ell \ .$$

Thus if one fixes the number of particles in the system, fixes the density of the system, and calculates the eigenvalues of H consistent with these two constraints, a sequence of ordered energy eigenvalues $E_o \leq E_1 \leq \cdots \leq E_j \leq E_{j+1} \leq \ldots$ may be obtained. A change in the number of particles or the density of particles can be expected to change these energy eigenvalues. Let $E_\alpha(N)$ be the eigenvalue of H corresponding to the eigenstate $|N,\alpha\rangle$, that is,

$$H\,|N,\alpha\rangle = E_\alpha(N)\,|N,\alpha\rangle ,$$

where α orders the eigenvalues so that

$$E_\alpha(N) \leq E_{\alpha+1}(N) .$$

Note that the density dependence of $|N,\alpha\rangle$ and consequently $E_\alpha(N)$ has been omitted in this notation.

The Green's functions to be utilized in this work are defined by

$$G_j(\ell t) = -i\langle N_o,0|\,T\,[b_\ell^+(t)]^{j-1}\,[b_\ell(t)]^j\,b_o^+(0)\,|N_o,0\rangle \quad , \qquad j = 1,2,3,\ldots\ldots \tag{20}$$

where T is a time ordering operator such that

$$T\,[b_\ell^+(t)]^{j-1}\,[b_\ell(t)]^j\,b_o^+(0) = \left\{ \begin{array}{l} \Theta(t)\;[b_\ell^+(t)]^{j-1}\,[b_\ell(t)]^j\,b_o^+(0) \\ \\ +\Theta(-t)\;b_o^+(0)\,[b_\ell^+(t)]^{j-1}\,[b_\ell(t)]^j \end{array} \right\}$$

with

$$\Theta(t) = \left\{ \begin{array}{ll} 1 & \text{for } t>0 \\ \\ 0 & \text{for } t<0 \end{array} \right\} .$$

The averaging state, $|N_o,0>$, indicated in Equation (20) is the N_o-particle state with lowest energy for a given density. We emphasize that for this state, regardless of the density, we have N_o particles in N_o cells and therefore

$$<n_\ell> = 1 .$$

As we shall see later in this chapter, the functions defined by Equation (20) describe the propagation of a disturbance in the systems. For classical systems the Green's functions describe the propagation of a disturbance through the medium. This analogy accounts for the association of the name Green's function with the function of Equation (20).

In the following discussion it will prove advantageous to define the operator

$$F_{\ell,j} = [b_\ell^+]^{j-1} [b_\ell]^{j-1} , \tag{21}$$

which may be written (see Appendix A) as:

$$F_{\ell,j} = \begin{cases} 1 & j=1 \\ n_\ell(n_\ell-1)\cdots(n_\ell-j+2) & j\geq 2 \end{cases} , \tag{22}$$

where n_ℓ is the cell occupancy operator. With this definition of $F_{\ell,j}$ the Green's functions defined earlier become

$$G_j(\ell,t) = -i <T\, F_{\ell,j}(t)\, b_\ell(t)\, b_o^+(0)> ,$$

where explicit indication of $|N_o,0>$ as the averaging state is omitted.

Let us also define the functions

$$G_j^-(\ell t) = -i\,\Theta(-t)\,\langle b_o^+(0)\; F_{\ell,j}(t)\; b_\ell(t)\rangle \tag{23}$$

and

$$G_j^+(\ell t) = -i\,\Theta(t)\,\langle F_{\ell,j}(t)\; b_\ell(t)\; b_o^+(0)\rangle\ , \tag{24}$$

so that

$$G_j(\ell t) = G_j^-(\ell t) + G_j^+(\ell t)\ .$$

We now introduce a complete set of states $|N,\alpha\rangle$ and expand G_j^- and G_j^+ to get

$$G_j^-(\ell t) = -i\,\Theta(-t)\sum_{N,\alpha}\langle N_o,0|\, b_o^+(0)\,|N,\alpha\rangle\langle N,\alpha|\, F_{\ell,j}(t)\; b_\ell(t)\,|N_o,0\rangle \tag{25}$$

$$G_j^+(\ell t) = -i\,\Theta(t)\sum_{N,\alpha}\langle N_o,0|\, F_{\ell,j}(t)\; b_\ell(t)\,|N,\alpha\rangle\langle N,\alpha|\, b_o^+(0)\,|N_o,0\rangle\ . \tag{26}$$

Now write the cell operators utilizing the Heisenberg representation (in units such that $\hbar = 1$),

$$b_\ell(t) = e^{iHt}\; b_\ell\; e^{-iHt}$$

$$b_\ell^+(t) = e^{iHt}\; b_\ell^+\; e^{-iHt}$$

$$F_{\ell,j}(t) = e^{iHt}\; F_{\ell,j}\; e^{-iHt}\ ,$$

so that

$$\langle N_o,0|\, b_o^+(0)\,|N,\alpha\rangle = \langle N_o,0|\, b_o^+\,|N_o-1,\alpha\rangle\;\delta_{N,N_o-1} \tag{27}$$

$$\langle N,\alpha|\, F_{\ell,j}(t)\, b_\ell(t)\,|N_o,0\rangle = \langle N_o-1,\alpha|\, F_{\ell,j}\; b_\ell\,|N_o,0\rangle e^{-i[E_\alpha(N_o)-E_\alpha(N_o-1)]t}\delta_{N,N_o-1} \tag{28}$$

$$\langle N_o,0|\, F_{\ell,j}(t)\, b_\ell(t)\,|N,\alpha\rangle = \langle N_o,0|\, F_{\ell,j}\; b_\ell\,|N_o+1,\alpha\rangle e^{-i[E_\alpha(N_o+1)-E_o(N_o)]t}\delta_{N,N_o+1} \tag{29}$$

$$\langle N,\alpha|\, b_o^+(0)\,|N_o,0\rangle = \langle N_o+1,\alpha|\, b_o^+\,|N_o,0\rangle\, \delta_{N,N_o+1}\ , \tag{30}$$

where the particular values of N have been chosen consistent with the fact that b_o^+ adds a particle to the state upon which it acts, while $F_{\ell,j}\, b_\ell$ removes a particle. Substitution of Equation (27) through (30) into Equations (25) and (26) gives

$$G_j^-(\ell t) = -i\,\theta(-t)\sum_\alpha \langle N_o,0|\, b_o^+\,|N_o-1,\alpha\rangle\langle N_o-1,\alpha|\, F_{\ell,j}\, b_\ell\,|N_o,0\rangle\, e^{-i[E_o(N_o)-E_\alpha(N_o-1)]t} \tag{31}$$

$$G_j^+(\ell t) = -i\,\theta(t)\sum_\alpha \langle N_o,0|\, F_{\ell,j}\, b_\ell\,|N_o+1,\alpha\rangle\langle N_o+1,\alpha|\, b_o^+|N_o,0\rangle\, e^{-i[E_\alpha(N_o+1)-E_o(N_o)]t}\ .$$

Equations (22), (23), (24), (25), (26), and (31) permit physical interpretation of the Green's functions defined thus far. Consider first the case for $j = 1$. Equations (23), (24), and (31) are then

$$G_1^+(\ell t) = -i\,\theta(t)\,\langle N_o,0|\, b_\ell(t)\, b_o^+(0)\,|N_o,0\rangle \tag{32}$$

$$= -i\,\theta(t)\sum_\alpha \langle N_o,0|\, b_\ell\,|N_o+1,\alpha\rangle\langle N_o+1,\alpha|\, b_o^+\,|N_o,0\rangle\, e^{-i[E_\alpha(N_o+1)-E_o(N_o)]t}$$

$$G_1^-(\ell t) = -i\,\theta(-t)\,\langle N_o,0|\, b_o^+(0)\, b_\ell(t)\,|N_o,0\rangle \tag{33}$$

$$= -i\,\theta(-t)\sum_\alpha \langle N_o,0|\, b_o^+\,|N_o-1,\alpha\rangle\langle N_o-1,\alpha|\, b_\ell\,|N_o,0\rangle\, e^{-i[E_o(N_o)-E_\alpha(N_o-1)]t}\ .$$

From Equation (32) we see that $G_1^+(\ell t)$ relates to the occurrence of the following events:

(a) The creation of an $(N_o + 1)$-particle state from the N_o-particle ground state by the addition of a particle to cell 0 at $t = 0$.

(b) The subsequent return to the N_o-particle ground state by the removal of a particle from cell ℓ at the time t.

If the state $|N_o,0\rangle$ is such that these two events may occur with relatively high probability, then this is reflected by a relatively large magnitude for $G_1^+(\ell t)$. If, however, $|N_o,0\rangle$ is such that the probability for these two events is small, then we can expect a correspondingly small value for $G_1^+(\ell t)$.

We consider two examples chosen so that $G_1^+(\ell t)$ may be evaluated exactly in the high density limit (where we have seen that $H \simeq V$). First consider the completely localized state, $|n_j = 1\rangle$, which we have seen to be the ground state of H for very high densities. Now

$$b_o^+(0)\,|m_j=1\rangle = b_o^+\,|m_j=1\rangle = \sqrt{2}\,|m_j=1+\delta_{jo}\rangle ,$$

and

$$\begin{aligned} b_\ell^+(t)\,|m_j=1\rangle &= e^{iHt}\, b_\ell^+\, e^{-iHt}\,|m_j=1\rangle \\ &= e^{iVt}\, b_\ell^+\, e^{-iVt}\,|m_j=1\rangle \\ &= e^{iVt}\, b_\ell^+\,|m_j=1\rangle \\ &= e^{iVt}\,\sqrt{2}\,|m_j=1+\delta_{j\ell}\rangle \\ &= \sqrt{2}\, e^{ip u_o t}\,|m_j=1+\delta_{j\ell}\rangle . \end{aligned}$$

Therefore

$$\begin{aligned} G_1^+(\ell t) &= -i\,\theta(t)\; 2\, e^{-ip u_o t}\,\langle m_j=1+\delta_{j\ell}\,|\,m_j=1+\delta_{jo}\rangle \\ &= -2i\,\theta(t)\, e^{-ip u_o t}\,\delta_{\ell,o} . \end{aligned}$$

Thus we see that unless the particle addition and subsequent particle removal occur within the same cell, it is impossible to return to the

initial state. The frequency of oscillation, ρU_o, corresponds to the energy difference between the initial state $|n_j = 1\rangle$ with energy zero and the intermediate state $|n_j = 1 + \delta_{j_o}\rangle$ with energy ρU_o.

As a second example let us use as the averaging state the $(N_o + 1)$-particle state

$$|N_o+1, k\rangle = \frac{1}{\sqrt{N_o}} \sum_m e^{\frac{2\pi i\, k\cdot m}{2N+1}} \; |m_j = 1 + \delta_{jm}\rangle \;, \tag{34}$$

which consists of a superposition of states having two particles in cell m and one particle in the remaining cells. It should be noted that for this illustration, we are relaxing the requirement that the averaging state be an N_o-particle state. That the states represented by Equation (34) are orthogonal for different values of k and normalized is seen by

$$\begin{aligned}
\langle N_o+1, k' | N_o+1, k\rangle &= \frac{1}{N_o} \sum_{m'} \sum_m e^{\frac{2\pi i\,(k\cdot m - k'\cdot m')}{2N+1}} \langle m_j = 1+\delta_{jm'} | m_j = 1+\delta_{jm}\rangle \\
&= \frac{1}{N_o} \sum_{m'} \sum_m e^{\frac{2\pi i\,(k\cdot m - k'\cdot m')}{2N+1}} \delta_{m',m} \\
&= \frac{1}{N_o} \sum_m e^{\frac{2\pi i\,(k-k')\cdot m}{2N+1}} = \delta_{k',k} \,.
\end{aligned}$$

Now (again at high densities so that $H \simeq V$),

$$\begin{aligned}
b_o^+(0)\,|N_o+1, k\rangle &= \frac{1}{\sqrt{N_o}} \sum_m e^{\frac{2\pi i\, k\cdot m}{2N+1}} \; b_o^+ \; |m_j = 1+\delta_{jm}\rangle \\
&= \frac{1}{\sqrt{N_o}} \sum_m e^{\frac{2\pi i\, k\cdot m}{2N+1}} \; \sqrt{2+\delta_{m,o}} \; |m_j = 1+\delta_{jm}+\delta_{jo}\rangle,
\end{aligned}$$

and

$$b_\ell^+(t)\,|N_0+1,k\rangle = \frac{1}{\sqrt{N_0}}\sum_m e^{\frac{2\pi i k\cdot m}{2N+1}}\, e^{iVt}\, b_\ell^+\, e^{-iVt}\,|m_j = 1+\delta_{jm}\rangle$$

$$= \frac{1}{\sqrt{N_0}}\sum_m e^{\frac{2\pi i k\cdot m}{2N+1}}\, e^{-ip u_0 t}\, e^{iVt}\, b_\ell^+\,|m_j = 1+\delta_{jm}\rangle$$

$$= \frac{1}{\sqrt{N_0}}\sum_m e^{\frac{2\pi i k\cdot m}{2N+1}}\, e^{-ip u_0 t}\sqrt{2+\delta_{\ell m}}\, e^{iVt}\,|m_j = 1+\delta_{jm}+\delta_{j\ell}\rangle$$

$$= \frac{1}{\sqrt{N_0}}\sum_m e^{\frac{2\pi i k\cdot m}{2N+1}}\, e^{i(1+\delta_{\ell m})p u_0 t}\sqrt{2+\delta_{\ell m}}\,|m_j = 1+\delta_{jm}+\delta_{j\ell}\rangle.$$

Therefore

$$G_1^+(\ell t) = -\frac{i\Theta(t)}{N_0}\sum_{m'}\sum_m e^{\frac{2\pi i k\cdot(m-m')}{2N+1}}\, e^{-i(1+\delta_{\ell m'})t}\sqrt{2+\delta_{\ell m'}}\sqrt{2+\delta_{\ell m}}$$

$$\times\langle m_j = 1+\delta_{jm'}+\delta_{j\ell}\,|\,m_j = 1+\delta_{jm}+\delta_{j0}\rangle.$$

But

$$\langle m_j = 1+\delta_{jm'}+\delta_{j\ell}\,|\,m_j = 1+\delta_{jm}+\delta_{j0}\rangle = \delta_{m'm}\delta_{\ell 0}+\delta_{\ell m}\delta_{m'0}-\delta_{\ell m}\delta_{mm'}\delta_{m0}$$

so that

$$G_1^+(\ell t) = -i\Theta(t)\Big[\frac{2}{N_0}\sum_{m\neq 0} e^{-ip u_0 t}\,\delta_{\ell 0}+\frac{2}{N_0}\sum_{m\neq 0} e^{\frac{2\pi i k\cdot m}{2N+1}}\, e^{-ip u_0 t}\,\delta_{\ell m}+\frac{3}{N_0}e^{-2ip u_0 t}\,\delta_{\ell 0} \qquad (35)$$

$$= -i\Theta(t)\Big[2\Big(\frac{N_0-1}{N_0}\Big)\, e^{-ip u_0 t}\,\delta_{\ell 0}+\frac{3}{N_0}\, e^{-2ip u_0 t}\,\delta_{\ell 0}+\frac{2}{N_0}e^{\frac{2\pi i k\cdot\ell}{2N+1}}\, e^{-ip u_0 t}(1-\delta_{\ell 0})\Big].$$

Let us rewrite Equation (35) as

$$G_1^+(0,t) = -i\Theta(t)\Big[2\Big(\frac{N_0-1}{N_0}\Big)\, e^{-ip u_0 t}+\frac{3}{N_0}\, e^{-2ip u_0 t}\Big] \qquad (36)$$

$$G_1^+(\ell\neq 0,t) = -i\,\Theta(t)\,\frac{2}{N_0}\, e^{\frac{2\pi i k\cdot\ell}{2N+1}}\, e^{-ip u_0 t}\,. \qquad (37)$$

$G_1^+(0,t)$ relates, of course, to the creation of a particle in cell zero and the destruction of a particle in the same cell a time t later. This can occur via two distinctly different processes:

(a) Cell zero has a single occupant, the double occupancy occurring at one of the $(N_o - 1)$ other cells. The resulting intermediate state is one with two double occupancies.

(b) Cell zero is doubly occupied. The resulting intermediate state is one with a triply occupied cell.

For case (a), returning to the initial state by destruction in cell zero results in the first term of Equation (36), where the $(N_o - 1)$ multiplicative factor reflects the number of possible sites for the original doubly occupied cell. The initial state corresponds to an energy of ρU_o while the intermediate state has an energy of $2\rho U_o$, giving the ρU_o frequency associated with this term. For case (b), which can occur for only one of the superposed states of Equation (34), the intermediate state has an energy $3\rho U_o$, and thus the frequency for this case is $2\rho U_o$ as seen in the second term of Equation (36).

Now $G_1^+(\ell \neq 0,t)$ relates to the creation of a particle in cell zero and the subsequent destruction of a particle in cell ℓ. This process occurs in the following manner. The b_o^+ operator creates a double at cell zero in the $m = \ell$ member of Equation (34) which has a double at cell ℓ. The subsequent removal of a particle from cell ℓ returns this state to one identical to a second member of the original set; this secong member being the one with a double occupancy in cell zero. Hence, a nonzero matrix element for the process results. The intermediate

state consists of two doubles with an energy of $2\rho U_o$, and therefore accounts for the frequency ρU_o of Equation (37).

We see that $G_1^+(\ell t)$ is the probability amplitude for taking the system in a specified state (the lowest energy state in our case), adding a particle to the system at some selected location, removing a particle a distance ℓ away and a time t later, and returning to the initial state. If the averaging state is completely localized, as in the first example, then the particle removal must occur at the same location as the particle addition. As a consequence of this localization of the averaging state, $G_1^+(\ell t)$ demonstrates a localization, that is, it is zero except for $\ell = 0$. The averaging state in the second example superposes states, which individually exhibit a high degree of localization, in such a manner that a possibility of other than single occupancy occurs for each cell. This slight delocalization of the averaging state is reflected by a $G_1^+(\ell t)$ which, although still a maximum for $\ell = 0$, is no longer zero for $\ell \neq 0$. Thus for the cell model as the density of the system decreases, increased particle movement will be reflected in increased magnitudes for $G_1^+(\ell t)$ for $\ell \neq 0$.

Similarly

$$G_1^-(\ell t) = -i\Theta(-t)\langle N_0, 0 | b_0^+(0)\, b_\ell(t) | N_0, 0\rangle$$

is the probability amplitude for removing a particle from the ground state, adding a particle to the system a distance ℓ away and a time $|-t|$ later, and returning to the ground state. We expect $G_1^-(\ell t)$ to reflect the state of localization of the ground state in the same manner as $G_1^+(\ell t)$.

With the detailed discussion of $G_1^{\pm}(\ell t)$ we turn briefly to a consideration of higher order Green's functions. Since

$$F_{\ell,j}(t)\, b_\ell(t) = [b_\ell^+(t)]^{j-1}\, [b_\ell(t)]^j$$

destroys j particles in cell ℓ and immediately returns $(j-1)$ of these to the cell, the net effect is to remove one particle from cell ℓ at the time t. In this respect it is similar to the operator $b_\ell(t)$. It differs in that for an ℓ cell occupancy of $j-1$, or less, the j successive removals result in a null result, i.e.,

$$F_{\ell,j}\, b_\ell \,|\, n_\ell < j \rangle = 0 .$$

Therefore $(j > 1)$

$$G_j^+(\ell t) = -i\,\theta(t) \langle F_{\ell,j}(t)\, b_\ell(t)\, b_o^+(0) \rangle$$

relates, just as does $G_1^+(\ell t)$, to the addition of a particle to the ground state and the subsequent removal of a particle (at a time t and a displacement ℓ) to return to the ground state. These functions differ from $G_1^+(\ell t)$ in that the amplitude of the disturbance is "modulated" by a fluctuation associated with cell ℓ after removal of one particle. Likewise

$$G_j^-(\ell t) = -i\,\theta(-t) \langle b_o^+(0)\, F_{\ell,j}(t)\, b_\ell(t) \rangle$$

for $j > 1$ is similar to $G_1^-(\ell t)$ in that it relates to a particle removal followed in time by a particle addition, and differs from $G_1^-(\ell t)$ in that the amplitude of this disturbance is modulated by a fluctuation.

To expand on this difference between $G_j(\ell t)$ and $G_1(\ell t)$, suppose we approximate the N_0-particle ground state by the best-possible superposition of states disgonal in occupation number space subject to the constraint that no cell occupancy exceed two. Let such an approximation be denoted by $|2\rangle$. Now $b_\ell^3|2\rangle \equiv 0$ so that

$$G_3^-(\ell t) = -i\theta(-t)\langle 2|\, b_0^+(0)\left[b_2^+(t)\right]^2\left[b_1(t)\right]^3|2\rangle \equiv 0 \ ,$$

while

$$G_3^+(\ell t) = -i\theta(t)\langle 2|\left[b_2^+(t)\right]^2\left[b_1(t)\right]^3 b_0^+(0)\,|2\rangle$$

$$= -i\,\theta(t)\langle 2|\left[b_0^+(t)\right]^2\left[b_0(t)\right] b_0^+(0)\,|2\rangle\,\delta_{\ell 0} \ ,$$

and

$$G_j^-(\ell t) = G_j^+(\ell t) \equiv 0 \qquad \text{for } j>3 \ .$$

We conclude that for a ground state with small fluctuations away from the localized state, the Green's functions for increasing j demonstrate a decreasing magnitude.

Until now the remarks of this chapter concerning the Green's functions defined herein have been, for the most part, concerned with interpretation on the basis of spatial considerations. While this interpretation is of basic importance if one is to utilize the Green's function formalism to its fullest measure, we shall see that a second essential feature of interest in this work is related to the energy difference appearing as frequencies in the expansions of equations (31). For a consideration of these quantities we utilize the chemical potential introduced in the previous chapter. Now

$$E_o(N_o) - E_\alpha(N_o-1) = E_o(N_o) - E_\alpha(N_o-1) + E_\alpha(N_o-1) - E_\alpha(N_o-1) \tag{38}$$

$$= \mu^- - \varepsilon(N_o-1,\alpha) \quad ,$$

where

$$\varepsilon(N_o-1,\alpha) = E_\alpha(N_o-1) - E_o(N_o-1) \tag{39}$$

is the excitation energy associated with the state $|N_o - 1, \alpha\rangle$. Similarly

$$E_\alpha(N_o+1) - E_o(N_o) = E_\alpha(N_o+1) - E_o(N_o+1) + E_o(N_o+1) - E_o(N_o) \tag{40}$$

$$= \varepsilon(N_o+1,\alpha) + \mu^+ \quad ,$$

where

$$\varepsilon(N_o+1,\alpha) = E_\alpha(N_o+1) - E_o(N_o+1) \tag{41}$$

is the excitation energy associated with the state $|N_o + 1, \alpha\rangle$. With Equations (38) and (40), Equations (31) become

$$G_j^-(\ell t) = -i\,\Theta(t) \sum_\alpha \langle N_o,0|\, b_o^+ \,|N_o-1,\alpha\rangle \langle N_o-1,\alpha|\, F_{\ell,j}\, b_\ell \,|N_o,0\rangle\, e^{-i[\mu^- - \varepsilon(N_o-1,\alpha)]t} \tag{42}$$

$$G_j^+(\ell t) = -i\,\Theta(t) \sum_\alpha \langle N_o,0|\, F_{\ell,j}\, b_\ell \,|N_o+1,\alpha\rangle \langle N_o+1,\alpha|\, b_o^+ \,|N_o,0\rangle\, e^{-i[\mu^+ + \varepsilon(N_o+1,\alpha)]t} \quad . \tag{43}$$

Three important observations follow from Equations (42) and (43).

1. All $G_j^-(\ell t)$ functions exhibit the same frequencies, namely

$$\omega^-(\alpha) = \mu^- - \varepsilon(N_o-1,\alpha) \quad ,$$

with the j-difference occurring in the amplitude, $\langle N_o,0|\, b_o^+ |N_o - 1, \alpha\rangle \langle N_o - 1, \alpha|\, F_{\ell,j}\, b_\ell |N_o,0\rangle$, associated with these frequencies. Similarly

all $G_j^+(\ell t)$ functions possess the same frequencies,

$$\omega^+(\alpha) = \mu^+ + \varepsilon(N_o+1,\alpha)$$

with the j-differences being observed in the amplitudes $\langle N_o, 0|F_{\ell,j}\, b_\ell|N_o+1, \alpha\rangle\langle N_o+1, \alpha|b_o^+|N_o, 0\rangle$. Since the excitation energies in both cases are nonnegative, it follows that

$$\omega^-(\alpha) \leq \omega^-_{MAX} = \mu^- \tag{44}$$

and

$$\omega^+(\alpha) \geq \omega^+_{MIN} = \mu^+ \quad . \tag{45}$$

2. Now μ^+ can be interpreted as the energy added to the system by adding a particle to the N_o-particle ground state, whereas μ^- may be considered as the energy removed from the system by subtracting a particle from the N_o-ground state to create the $(N_o - 1)$-ground state. For high densities we have already seen that the cell model exhibits characteristics peculiar to the solid in that the particles are localized one to a cell and held there by the large repulsive potential interaction. Therefore the addition of a particle anywhere in the system requires the addition of a large amount of energy since, necessarily, the particle must be placed in an already occupied cell. The energy lost by removing a particle from this state is considerably less, since removing a particle from a singly occupied cell costs no potential energy in this model. As the density decreases, the particle wanderings produced by the energy lowering effect of the off-diagonal (in occupation number space) kinetic energy operator render this distinction between particle addition and

particle removal less discernible. As long as the system retains its solid identity, i.e., small fluctuations away from the localized state, we expect this distinction to occur. Therefore

$$\mu^- < \mu^+ \qquad \text{(solid)}. \tag{46}$$

For an arbitrary system in the liquid state since particles are relatively free to adjust their configuration, the difference in μ^+ and μ^- should be attributable to the slightly different volume per particle in the N_o and $N_o + 1$ states. Since

$$\Delta v = \frac{V}{N_o} - \frac{V}{N_o+1} = \frac{V}{N_o(N_o+1)} \simeq \frac{V}{N_o^2} = \frac{v}{N_o} ,$$

where v is the volume per particle, we expect that for the liquid

$$0 < \mu^+ - \mu^- \sim \mathcal{O}(1/N_o) \qquad \text{(liquid)}.$$

It is precisely this characteristic of a liquid which we shall employ as a signal to recognize an apparent solid-liquid transition in the cell model of this work.

3. With Equations (44), (45), and (46) we see that for the solid

$$\omega^-(\alpha) \leq \omega^-_{MAX} = \mu^- < \mu^+ = \omega^+_{MIN} \leq \omega^+(\alpha) . \tag{47}$$

The point to be emphasized here is that

$$\omega^-_{MAX} < \omega^+_{MIN} . \tag{48}$$

The arguments leading to Equation (48) follow only if we require the averaging state to be the ground state of the system. We shall find in

later chapters that this point plays a most vital role in the solution of the equations of motion of the Green's functions.

Another property of the Green's functions which will be incorporated into the solution of the equations of motion is a discontinuity which exists in $G_j(\ell t)$ at $t = 0$. Note that $G_j(\ell t)$ is not defined for this time. Consider the limiting process

$$\lim_{t\to 0^+} iG_j(\ell t) - \lim_{t\to 0^-} iG_j(\ell t) = \langle F_{\ell,j}\, b_\ell\, b_o^+ - b_o^+ F_{\ell,j}\, b_\ell \rangle = \langle [F_{\ell j}\, b_\ell,\, b_o^+] \rangle \ .$$

For $j \geq 2$

$$\begin{aligned}[F_{\ell,j}\, b_\ell,\, b_o^+] &= (b_\ell^+)^{j-1} (b_\ell)^j b_o^+ - b_o^+ (b_\ell^+)^{j-1} (b_\ell)^j \\ &= j\,(b_\ell^+)^{j-1} (b_\ell)^{j-1} \delta_{\ell,0} = j\,(b_o^+)^{j-1} (b_o)^{j-1} \delta_{\ell,0} \\ &= j\ m_o(m_o-1)\cdots(m_o-j+2)\,\delta_{\ell,0} \ ,\end{aligned}$$

while for $j = 1$

$$[F_{\ell,1}\, b_\ell,\, b_o^+] = b_\ell b_o^+ - b_o^+ b_\ell = \delta_{\ell,0} \ .$$

Thus we have

$$\lim_{t\to 0^+} iG_j(\ell t) - \lim_{t\to 0^-} iG_j(\ell t) = j\,\Delta_j\,\delta_{\ell,0} \ , \tag{49}$$

where

$$\Delta_j = \begin{cases} 1 & j = 1 \\ \langle m_o(m_o-1)\cdots(m_o-j+2) & j \geq 2 \end{cases} . \tag{50}$$

Furthermore

$$\lim_{t\to 0^-} i G_j(\ell=0,t) = \langle b_o^+ F_{o,j}\, b_\ell \rangle = \langle (b_o^+)^{j+1} (b_o)^j \rangle = \Delta_{j+1} , \tag{51}$$

so that for $j \geq 2$ Equation (49) may be written

$$\lim_{t\to 0^+} G_j(\ell,t) - \lim_{t\to 0^-} G_j(\ell,t) = j \lim_{t\to 0^-} G_{j-1}(\ell=0,t)\, \delta_{\ell,0} .$$

Equation (51) should be particularly noted for $j = 1$, in which case

$$\lim_{t\to 0^-} i G_1(\ell=0,t) = \langle b_o^+ b_o \rangle = \langle n_o \rangle .$$

Since we are requiring the cell sizes to vary with density such that for the N_o-particle system, which is the averaging state, the average number of particles per cell is exactly unity, we have

$$\lim_{t\to 0^-} i G_1(\ell=0,t) = 1 . \tag{52}$$

Green's Function Equation of Motion

The arguments of the past few paragraphs have pointed out the importance of the time varying portion of the Green's functions. We have seen that a knowledge of the two sets of frequencies, $\omega^-(\alpha)$ and $\omega^+(\alpha)$, associated with these functions allow (a) a calculation of μ^+ and μ^- and hence an identification as to whether the system for a specified density is in the solid or liquid state; and (b) a calculation of $\varepsilon(N_o + 1, \alpha)$ and $\varepsilon(N_o - 1, \alpha)$, which represent the energy excitation spectrum for the system.

We conclude that a solution for the time dependence of these functions would yield a bountiful supply of information, both

microscopic and macroscopic, about the system. In order to attempt such a solution in later chapters we will need the differential equations in t (herein called the equations of motion) which the Green's functions obey. As the concluding effort of this chapter we obtain these equations.

Differentiating $G_j(\ell t)$ with respect to t, we obtain $(t \neq 0)$.

$$i \frac{\partial G_j(\ell t)}{\partial t} = \langle T \frac{\partial}{\partial t} [F_{\ell,j}(t) b_\ell(t)] b_0^+(0) \rangle .$$

Now the time rate of change of an arbitrary operator $O(t)$ with no explicit time dependence is given by

$$\frac{dO(t)}{dt} = -i [O(t), H(t)] ,$$

where H is the Hamiltonian of the system. Therefore

$$\frac{\partial}{\partial t} [F_{\ell,j}(t) b_\ell(t)] = -i [F_{\ell,j}(t) b_\ell(t), H(t)] ,$$

so that

$$i \frac{\partial G_j(\ell t)}{\partial t} = -i \langle T [F_{\ell,j}(t) b_\ell(t), H(t)] b_0^+(0) \rangle .$$

In Appendix (B) we demonstrate that

$$[F_{\ell,j} b_\ell, H] = \left\{ \begin{array}{l} [(j-1)\rho U_0 + \sigma K] F_{\ell,j} b_\ell + \rho U_0 F_{\ell,j+1} b_\ell \\ -jK \sum_{r'} F_{\ell,j} b_{\ell+r'} + (j-1) K \sum_{r'} b^+_{\ell+r'} F_{\ell,j-1} b_\ell b_\ell \end{array} \right\} ,$$

so that

$$i \frac{\partial G_j(\ell t)}{\partial t} = \left\{ \begin{array}{l} -i [(j-1)\rho U_0 + \sigma K] \langle T F_{\ell,j}(t) b_\ell(t) b_0^+(0) \rangle - i \rho U_0 \langle T F_{\ell,j+1}(t) b_\ell(t) b_0^+(0) \rangle \\ + i j K \sum_{r'} \langle T F_{\ell,j}(t) b_{\ell+r'}(t) b_0^+(0) \rangle - i (j-1) K \sum_{r'} \langle T b^+_{\ell+r'}(t) F_{\ell,j-1}(t) b_\ell(t) b_\ell(t) b_0^+(0) \rangle \end{array} \right\} .$$

But

$$-i\langle T F_{\ell,j}(t)\, b_\ell(t)\, b_0^+(0)\rangle = G_j(\ell t)\ ,$$

and

$$-i\langle T F_{\ell,j+1}(t)\, b_\ell(t)\, b_0^+(0)\rangle = G_{j+1}(\ell t)\ ;$$

and so

$$\left[i\frac{\partial}{\partial t} - 6K - (j-1)\rho U_0\right] G_j(\ell t) = -jK D_j(\ell t) + (j-1)K E_j(\ell t) + \rho U_0 G_{j+1}(\ell t) \qquad (53)$$

where

$$D_j(\ell t) = -i \sum_{r'} \langle T F_{\ell,j}(t)\, b_{\ell+r'}(t)\, b_0^+(0)\rangle \qquad (54)$$

$$E_j(\ell t) = -i \sum_{r'} \langle T b_{\ell+r'}^+(t)\, F_{\ell,j-1}(t)\, b_\ell(t)\, b_\ell(t)\, b_0^+(0)\rangle\ . \qquad (55)$$

CHAPTER IV

HIGH DENSITY APPROXIMATIONS IN THE GREEN'S FUNCTION EQUATIONS OF MOTION

In Chapter III we demonstrated the equation of motion for the function G_j to be

$$\left[i\frac{\partial}{\partial t} - \omega K - (j-1)\rho U_0\right] G_j(\ell t) = -jK D_j(\ell t) + (j-1)K E_j(\ell t) + \rho U_0 G_{j+1}(\ell t),$$

where

$$D_j(\ell t) = -i \sum_{r'} \langle T\,[b_\ell^\dagger(t)]^{j-1}\,[b_\ell(t)]^{j-1}\, b_{\ell+r'}(t)\, b_0^\dagger(0)\rangle$$

$$E_j(\ell t) = -i \sum_{r'} \langle T\, b_{\ell+r'}^\dagger(t)\, [b_\ell^\dagger(t)]^{j-2}\,[b_\ell(t)]^{j}\, b_0^\dagger(0)\rangle .$$

This set of coupled differential equations is exact for the cell-model Hamiltonian.

It should be noted here that for a system with a finite number of particles these equations are finite in number. To understand this, recall that the averaging state employed in the definition of G_j is the ground state for N_0 particles. Consider

$$G_{N_0+2}(\ell t) = -i \langle T\,[b_\ell^\dagger(t)]^{N_0+1}\,[b_\ell(t)]^{N_0+2}\, b_0^\dagger(0)\rangle \tag{56}$$

$$= \begin{cases} -i\,\Theta(t) \langle [b_\ell^\dagger(t)]^{N_0+1}\,[b_\ell(t)]^{N_0+2}\, b_0^\dagger(0)\rangle \\ \\ -i\,\Theta(-t) \langle b_0^\dagger(0)\,[b_\ell^\dagger(t)]^{N_0+1}\,[b_\ell(t)]^{N_0+2}\rangle \end{cases}$$

Now the maximum number of particles within any cell is N_o (in the averaging state) so that the $t < 0$ term of Equation (56) vanishes since $[b_\ell]^{N_o+2}$ operating on a cell of occupancy less than $(N_o + 2)$ yields zero. In the $t > 0$ term the b_o^+ operator makes the maximum occupancy of cell number zero $(N_o + 1)$. As before, the $(N_o + 2)$ successive applications of b_ℓ still yields zero. Thus

$$G_{N_o+2}(\ell t) \equiv 0 \ ,$$

and the terminating equation is

$$\left(i\frac{\partial}{\partial t} - 6K - N_o\rho U_o\right) G_{N_o+1}(\ell t) = -(N_o+1)K\, D_{N_o+1}(\ell t) + (N_o-1)K\, E_{N_o+1}(\ell t) \ .$$

Even with the simplification of the previous paragraph, the system of differential equations is still complicated by the presence of the D_j and E_j functions. Since these functions cannot be expressed in terms of the G_j functions, their presence in the differential equations rule out any exact solution for G_j from these equations of motion alone. A possible procedure at this point would be to seek equations of motion for D_j and E_j. However, such an endeavor introduces additional difficulties. In particular, new and spatially more involved functions arise which themselves require equations of motion. This most difficult situation makes it advisable to treat the D_j and E_j functions in a different manner.

Arguments in Chapter II demonstrated that for sufficiently high densities the parameter K is much less than ρU_o. Now D_j and E_j appear in the G_j equation of motion with K as a multiplicative coefficient. Therefore we expect the contribution from these terms to be

small for reasonably high densities. Thus if we approximate D_j and E_j by judicious combinations of G_j's, these approximations are being made on reasonably small terms. Such approximations are our objective in this chapter. The primary criterion which we shall employ is that all approximations shall be exact in the high density limit, which corresponds to the completely localized system.

The D_1 and E_1 functions require no approximations since

$$D_1(\ell t) = -i \sum_{r'} \langle T\, b_{\ell+r'}(t)\, b_0^+(0) \rangle = \sum_{r'} G_1(\ell+r', t) \;, \tag{57}$$

and since the coefficient multiplying E_1 in the G_1 equation of motion is zero. The first terms which must be approximated are

$$D_2(\ell t) = -i \langle T\, b_\ell^+(t)\, b_\ell(t) \sum_{r'} b_{\ell+r'}(t)\, b_0^+(0) \rangle \tag{58}$$

and

$$E_2(\ell t) = -i \langle T \sum_{r'} b_{\ell+r'}^+(t)\, b_\ell(t)\, b_\ell(t)\, b_0^+(0) \rangle \;. \tag{59}$$

Let

$$D_2^+(\ell t) = -i\, \Theta(t) \langle b_\ell^+(t)\, b_\ell(t) \sum_{r'} b_{\ell+r'}(t)\, b_0^+(0) \rangle \tag{60}$$

$$D_2^-(\ell t) = -i\, \Theta(-t) \langle b_0^+(0)\, b_\ell^+(t)\, b_\ell(t) \sum_{r'} b_{\ell+r'}(t) \rangle \;, \tag{61}$$

so that

$$D_2(\ell t) = D_2^+(\ell t) + D_2^-(\ell t) \;. \tag{62}$$

For the localized system ($|n_j = 1\rangle$), which is the ground state in the high density limit,

$$b_\ell^+(t)\, b_\ell(t)\, |m_j = 1\rangle = |m_j = 1\rangle \;,$$

and so in this limit

$$b_\ell^+(t)\, b_\ell(t)\, |N_0, 0\rangle \longrightarrow |N_0, 0\rangle \ .$$

Therefore as the system approaches the localized state,

$$D_2^+(\ell t) = -i\,\Theta(t) \langle b_\ell^+(t)\, b_\ell(t) \sum_{r'} b_{\ell+r'}(t)\, b_0^+(0)\rangle$$

$$\longrightarrow -i\,\Theta(t) \sum_{r'} \langle b_{\ell+r'}(t)\, b_0^+(0)\rangle \ ,$$

or

$$D_2^+(\ell t) \simeq \sum_{r'} G_1^+(\ell+r', t) \ . \tag{63}$$

Similarly

$$D_2^-(\ell t) = -i\,\Theta(-t) \langle b_0^+(0) \sum_{r'} b_{\ell+r'}(t)\, b_\ell^+(t)\, b_\ell(t)\rangle$$

$$\longrightarrow -i\,\Theta(-t) \langle b_0^+(0) \sum_{r'} b_{\ell+r'}(t)\rangle$$

or

$$D_2^-(\ell t) \simeq \sum_{r'} G_1^-(\ell+r', t) \ . \tag{64}$$

Equations (62), (63), and (64) give

$$D_2(\ell t) \simeq \sum_{r'} G_1(\ell+r', t) \tag{65}$$

as our approximation for D_2. Equation (65) is an example of what is usually called the Hartree approximation, in analogy with the Hartree approximation of quantum mechanics where a multiple-particle wave function is replaced by a product of single-particle wave functions. With Green's functions we replace a two-particle Green's function by a product of two single-particle Green's functions. To demonstrate this explicitly with D_2 we have

$$D_2(\ell t) = -i \langle T\, b_\ell^+(t)\, b_\ell(t) \sum_{r'} b_{\ell+r'}(t)\, b_0^+(0) \rangle$$

$$\simeq -i \langle b_\ell^+(t)\, b_\ell(t) \rangle \sum_{r'} \langle T\, b_{\ell+r'}(t)\, b_0^+(0) \rangle$$

$$= \sum_{r'} G_1(\ell+r', t) \ ,$$

which agrees with Equation (65). Caution must be exercised in such approximations since no general statement can be made about the validity of such estimates.

The Hartree approximation may be used for E_2 to get

$$E_2(\ell t) = -i \sum_{r'} \langle T\, b_{\ell+r'}^+(t)\, b_\ell(t)\, b_\ell(t)\, b_0^+(0) \rangle \tag{66}$$

$$\simeq -i \sum_{r'} \langle b_{\ell+r'}^+(t)\, b_\ell(t) \rangle \langle T\, b_\ell(t)\, b_0^+(0) \rangle$$

or

$$E_2(\ell t) \simeq g_2\, G_1(\ell t) . \tag{67}$$

where g_2 is a function of the density of the system. Equation (66) suggests that

$$g_2 = \sum_{r'} \langle b_{\ell+r'}^+\, b_\ell \rangle \ . \tag{68}$$

To demonstrate that this is not necessarily the best choice, consider the limiting procedure

$$i\, E_2(\ell, t=0^+) - i\, E_2(\ell, t=0^-) = \sum_{r'} \langle b_{\ell+r'}^+ b_\ell b_\ell b_0^+ - b_0^+ b_{\ell+r'}^+ b_\ell b_\ell \rangle . \tag{69}$$

With the commutation rules

$$[\, b_\ell,\ b_m^+ \,] = \delta_{\ell,m} \qquad [\, b_\ell^+,\ b_m^+ \,] = 0 \ ,$$

Equation (69) becomes

$$i E_2(\ell,t=0^+) - i E_2(\ell,t=0^-) = z \sum_{r'} \langle b_{\ell+r'} b_\ell^+ \rangle \delta_{\ell,0} . \tag{70}$$

From Equation (67)

$$i E_2(\ell,t=0^+) - i E_2(\ell,t=\sigma) = g_2 [i G_1(\ell,t=0^+) - i G_1(\ell,t=0^-)]$$

$$= g_2 \langle b_\ell b_0^+ - b_0^+ b_\ell \rangle$$

or

$$i E_2(\ell,t=0^+) - i E_2(\ell,t=0^-) = g_2 \delta_{\ell,0} . \tag{71}$$

A comparison of Equations (70) and (71) suggests that

$$g_2 = z \sum_{r'} \langle b_{\ell+r'} b_\ell^+ \rangle ,$$

in contrast with Equation (68).

In the high density limit $E_2(\ell t) = 0$ since the operators whose average define E_2 necessarily change the number of particles in cell ℓ resulting in a zero when averaged over the localized state. Since $G_1(\ell t)$ is not identically zero in this same limit, we conclude from Equation (67) that g_2 must vanish in the localized state. This consideration, coupled with the ambiguity presented in the previous paragraph for the best definition of g_2, suggests that the only requirement we should place on g_2 is that it approach zero in the high density limit. In Chapter VI we shall use this freedom of choice for g_2 to assist in assuring that solutions for certain Green's functions satisfy a normalization requirement.

Approximations for higher order D and E functions will be presented now with a few comments. We shall find, however, that the solutions presented in Chapter VI do not involve the resulting approximations. Even though these terminations play no role in the essential part of this particular endeavor, these approximations are presented as suggestions for possible future investigation. For the D functions we use a Hartree-like procedure to get

$$D_j(\ell t) = -i \langle T\,[b_2^\dagger(t)]^{j-1}\,[b_2(t)]^{j-1} \sum_{r'} b_{\ell+r'}(t)\; b_0^\dagger(0)\rangle$$

$$\simeq -i \langle [b_1^\dagger(t)]^{j-1}\,[b_1(t)]^{j-1}\rangle \sum_{r'} \langle T\, b_{\ell+r'}(t)\; b_0^\dagger(0)\rangle$$

or

$$D_j(\ell t) \simeq \Delta_j \sum_{r'} G_1(\ell+r', t)\,, \tag{72}$$

with

$$\Delta_j = \langle [b_1^\dagger]^{j-1}\,[b_1]^{j-1}\rangle\,.$$

Similarly

$$E_j(\ell t) = -i \langle T \sum_{r'} b_{\ell+r'}^\dagger(t)\; [b_1^\dagger(t)]^{j-2}\,[b_2(t)]^{j}\; b_0^\dagger(0)\rangle$$

$$\simeq -i \sum_{r'} \langle b_{\ell+r'}^\dagger(t)\; b_1(t)\rangle \langle T\,[b_2^\dagger(t)]^{j-2}\,[b_2(t)]^{j-1}\; b_0^\dagger(0)\rangle$$

or

$$E_j(\ell t) = g_j\; G_{j-1}(\ell t)\,, \tag{73}$$

where g_j (as with g_2) is an unspecified function of the density. Attempts to support these approximations for higher order D and E functions have been, for the most part, relatively unsuccessful, and consequently they are proposed here with some reservation.

With the approximations of Equations (65), (67), (72), and (73)

the equation of motion for G_j becomes

$$\left[i\frac{\partial}{\partial t} - 6K - (j-1)\rho U_o\right] G_j(\ell t) = -j\Delta_j K \sum_r G_1(\ell + r_j t) + (j-1) g_j K G_{j-1}(\ell t) + \rho U_o G_{j+1}(\ell t) \qquad (74)$$

for $1 \leq j \leq N_o + 1$

with

$$G_{N_o+2}(\ell t) \equiv 0 \quad .$$

If we divide Equation (74) by ρU_o, and recall the definition

$$\chi = 2K/\rho U_o \quad ,$$

we obtain, after rearrangement,

$$\frac{j\Delta_j \chi}{2} \sum_r G_1(\ell + r_j t) - (j-1)\frac{\chi g_j}{2} G_{j-1}(\ell t) + \left(\frac{i}{\rho U_o}\frac{\partial}{\partial t} - 3\chi - j + 1\right) G_j(\ell t) - G_{j+1}(\ell t) = 0 \quad . \qquad (75)$$

CHAPTER V

ON SOLVING THE EQUATIONS OF MOTION

In this chapter we give further consideration to the Green's functions' equations of motion obtained in Chapter IV and present a discussion as to what external information, if any, in the way of initial conditions is necessary to accomplish a solution.

The General Problem

The approximations of Chapter IV yield the following set of coupled differential equations of motion:

$$j\Delta_j \frac{\chi}{2} \sum_{r_1} G_1(l+r_j,t) - (j-1)q_j \frac{\chi}{2} G_{j-1}(lt) + \left(\frac{i}{\rho u_0}\frac{\partial}{\partial t} - 3\chi_{-j+1}\right) G_j(lt) + G_{j+1}(lt) = 0 \qquad (76)$$

for $1 \leq j \leq N_0 + 1$

with

$$G_{N_0+2}(lt) = 0 .$$

The $G_j(lt)$ obey the jump conditions:

$$i\left[G_j(l,t=0^+) - G_j(l,t=0^-)\right] = j\Delta_j \delta_{l,0} , \qquad (77)$$

where

$$\Delta_j = \left\{ \begin{array}{ll} 1 & j=1 \\ \langle m_l(m_l-1)\cdots(m_l-j+2)\rangle & j \geq 2 \end{array} \right\} .$$

Equations (76) may be simplified by introducing the Fourier transform

$$\mathcal{G}_j(kt) = \sum_{\ell} G_j(\ell t)\, e^{-\frac{2\pi i\, k\cdot\ell}{2N+1}} .$$

Multiplying by $e^{\frac{2\pi i k\cdot\ell'}{2N+1}}$ and summing on k gives

$$\sum_{k} \mathcal{G}_j(kt)\, e^{\frac{2\pi i k\cdot\ell'}{2N+1}} = \sum_{\ell} G_j(\ell t) \sum_{k} e^{\frac{2\pi i k\cdot(\ell'-\ell)}{2N+1}} ;$$

but

$$\sum_{k} e^{\frac{2\pi i k\cdot(\ell'-\ell)}{2N+1}} = N_0\, \delta_{\ell',\ell} ,$$

so that

$$G_j(\ell t) = \frac{1}{N_0} \sum_{k} \mathcal{G}_j(kt)\, e^{\frac{2\pi i k\cdot\ell}{2N+1}} . \tag{78}$$

Substituting Equation (78) into Equation (76) gives (after multiplying by N_0):

$$j\Delta_j \tfrac{x}{2} \sum_{k} \mathcal{G}_1(kt)\Big[\sum_{r'} e^{\frac{2\pi i k\cdot r'}{2N+1}}\Big] e^{\frac{2\pi i k\cdot\ell}{2N+1}} - (j-1) g_j \tfrac{x}{2} \sum_{k} \mathcal{G}_{j-1}(kt)\, e^{\frac{2\pi i k\cdot\ell}{2N+1}} \tag{79}$$

$$+ \Big(\tfrac{i}{\rho u_0}\tfrac{\partial}{\partial t} - 3x - j + 1\Big) \sum_{k} \mathcal{G}_j(kt) e^{\frac{2\pi i k\cdot\ell}{2N+1}} - \sum_{k} \mathcal{G}_{j+1}(kt)\, e^{\frac{2\pi i k\cdot\ell}{2N+1}} = 0 .$$

Multiplying Equation (79) by $e^{-\frac{2\pi i k\cdot\ell'}{2N+1}}$, summing over ℓ, and using

$$\sum_{\ell} e^{\frac{2\pi i (k-k')\cdot\ell}{2N+1}} = N_0\, \delta_{k,k'} ,$$

gives (letting $k = k'$):

$$j\Delta_j \cdot x\, S(k)\, \mathcal{G}_1(kt) - (j-1) g_j \tfrac{x}{2}\, \mathcal{G}_{j-1}(kt) + \Big(\tfrac{i}{\rho u_0} - 3x - j + 1\Big)\mathcal{G}_j(kt) - \mathcal{G}_{j+1}(kt) = 0 , \tag{80}$$

where

$$S(k) = \tfrac{1}{2} \sum_{r'} e^{\frac{2\pi i k\cdot r'}{2N+1}} = \sum_{i=1}^{3} \cos\tfrac{2\pi k_i}{2N+1} .$$

Comparison of Equations (80) with Equations (76) demonstrates the desirability of introducing the $\mathcal{G}_j(kt)$ functions in that the equations of motion for $G_j(\ell t)$ couple to $G_j(\ell + r', t)$ whereas those for $\mathcal{G}_j(kt)$ show no coupling between the different k-values.

The discontinuity at $t = 0$ in $G_j(\ell t)$ is transformed by multiplying Equation (77) by $e^{-\frac{2\pi i k\cdot\ell}{2N+1}}$ and summing on ℓ to get

$$i\left[\sum_{\ell} G_j(\ell, t=0^+)\, e^{-\frac{2\pi i k\cdot\ell}{2N+1}} - \sum_{\ell} G_j(\ell, t=0^-) e^{-\frac{2\pi i k\cdot\ell}{2N+1}}\right] = j\Delta_j \sum_{\ell} e^{-\frac{2\pi i k\cdot\ell}{2N+1}} \delta_{\ell,0}$$

or

$$i\left[\mathcal{G}_j(k, t=0^+) - \mathcal{G}_j(k, t=0^-)\right] = j\,\Delta_j . \tag{81}$$

The discussion in the next few paragraphs points out some of the general features involved in solving equations (80). The complexity of these equations prevents a complete solution, and therefore the latter portion of this chapter is devoted to further simplifications.

The characteristic equation for a system of equations of the type in Equation (80) is obtained by assuming solutions of the form

$$\mathcal{G}_j(kt) = A_j(k)\, e^{-\lambda \rho U_0 \nu t},$$

which, when substituted, yield the homogeneous algebraic system

$$j\Delta_j \times S(k)\, A_1(k) - (j-1) q_j \tfrac{\times}{2} A_{j-1}(k) + (\nu - 3\times - j + 1) A_j(k) - A_{j+1}(k) = 0,$$

for $1 \le j \le N_0 + 1$ with $A_{N_0+2}(k) \equiv 0$.

This system has a solution only if the characteristic polynomial $P_k(\nu)$, given in Equation (82), vanishes.

$$P_k(\nu) = \begin{vmatrix} \nu-3x+xS & -1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 2\Delta_2 xS - \frac{xg_3}{2} & \nu-3x-1 & -1 & 0 & \cdots & 0 & 0 & 0 \\ 3\Delta_3 xS & -xg_3 & \nu-3x-2 & -1 & \cdots & 0 & 0 & 0 \\ 4\Delta_4 xS & 0 & -\frac{3}{2}xg_4 & \nu-3x-3 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots \\ N_o\Delta_{N_o} xS & 0 & 0 & 0 & \cdots & -\frac{N_o-1}{2}xg_{N_o} & \nu-3x-N_o+1 & -1 \\ (N_o+1)\Delta_{N_o+1} xS & 0 & 0 & 0 & \cdots & 0 & -\frac{N_o}{2}xg_{N_o+1} & \nu-3x-N_o \end{vmatrix} \tag{82}$$

$P_k(\nu)$ is a polynomial of degree $N_o + 1$ in ν, resulting in $N_o + 1$ characteristic values $\nu_1(k)$, $\nu_2(k)$, ..., $\nu_{N_o+1}(k)$. The solution to the system of homogeneous differential equations of Equation (80) is (assuming the roots to be distinct)

$$i\mathcal{G}_j(kt) = \Theta(t)\sum_m a^+_{jkm} e^{-ip\mu_o\nu_m(k)t} + \Theta(-t)\sum_m a^-_{jkm} e^{-ip\mu_o\nu_m(k)t}, \tag{83}$$

where the constants a^+_{jkm} and a^-_{jkm} are to be determined. Let us determine the number of these coefficients for fixed k. The first subscript refers to the order of the Green's function and therefore ranges over $N_o + 1$ values. The third subscript indicates the characteristic root with which the coefficient is associated and hence ranges over $N_o + 1$ values. Thus we have $2(N_o + 1)^2$ coefficients for fixed k, the two arising since these coefficients must be determined for $t < 0$ and $t > 0$.

Substitution of Equations (83) into Equations (80) yields $N_o(N_o+1)$ independent equations for the a^+_{jkm} and an equal number for the a^-_{jkm}. Those equations, using the linear independence of the $e^{-i\nu_m(k)t}$ functions, are

$$j\Delta_j \times S\, a^{\pm}_{1km} - (j-1)g_j \tfrac{\chi}{2} a^{\pm}_{j-1,km} + [\nu_m(k) - 3\chi - j + 1]a^{\pm}_{jkm} - a^{\pm}_{j+1,km} = 0 \qquad (84)$$

for $1 \le j \le N_o$ and $1 \le m \le N_o + 1$.

The jump conditions of Equations (81), upon substitution of Equations (83), give

$$i\left[\sum_m a^+_{jkm} - \sum_m a^-_{jkm}\right] = j\Delta_j \qquad (85)$$

for $1 \le j \le N_o + 1$.

Equations (84) and (85) constitute $2N_o(N_o+1) + N_o + 1$ or $(2N_o+1)(N_o+1)$ equations for determining the $a^{\pm}_{jkm}$. We lack $2(N_o+1)^2 - (2N_o+1)(N_o+1)$ or (N_o+1) equations. These are the initial conditions

$$H_{jk} = i\,\mathcal{Y}_j(k, t=0^-) = \sum_m a^-_{jkm} \qquad (86)$$

for $1 \le j \le N_o + 1$. Thus it would appear that Equations (84), (85), and (86) permit a solution for the $2(N_o+1)^2$ constants for fixed k in terms of the (N_o+1) initial conditions H_{jk}. For the complete system since k ranges over N_o values, there are $2N_o(N_o+1)^2$ coefficients requiring $N_o(N_o+1)$ initial conditions.

The arguments presented above for determining the $\mathcal{Y}_j(kt)$ require a specification of $N_o(N_o+1)$ initial conditions and have, in no way

depended upon the earlier requirement that the averaging state in the definition of the $G_j(\ell t)$ be the ground state. Of course, any excited N_o-particle state could be chosen as the averaging state, and all of the arguments presented thus far in this chapter hold. This, then, accounts for the fact that we can specify the initial conditions without regard to the averaging state. A poor choice of initial conditions might, however, lead to no solution or perhaps a solution corresponding to using other than the ground state in the averaging. We seem to arrive at a difficult point, namely, that to determine the $\mathcal{B}_j(kt)$, or alternatively the $G_j(\ell t)$, we must have some means for specifying the initial conditions which assure the selection of the ground state as the averaging state. This difficulty is removed by using a result obtained in Chapter III. It is shown there that as a consequence of requiring the ground state as the averaging state, the frequencies appearing in the $t > 0$ portion of the solution are all greater than the maximum frequency occurring in the $t < 0$ portion. Returning to Equation (83), we see that this requires exactly one-half of the $2(N_o + 1)^2$ coefficients in this equation be zero, leaving only $(N_o + 1)^2$ to be determined for each value of k. With this new restriction Equations (84) yield $N_o(N_o + 1)$ equations while (85) still gives $N_o + 1$ equations. Therefore Equations (84) and (85) give $(N_o + 1)^2$ equations for determining the $(N_o + 1)^2$ constants, thereby completely removing the necessity of specifying the initial conditions of Equations (86). Thus we have, by using properties of $G_j(\ell t)$ determined in Chapter III, discovered an equivalent means for specifying the ground state as the

averaging state. One remark is necessary. We have not, as yet, submitted a prescription for determining just which frequencies correspond to the $t > 0$ solution and which to the $t < 0$ solution. The only requirement is that no frequency in the $t < 0$ solution shall exceed any frequency in the $t > 0$ solution. Later in this work when we are nearer an actual solution, we will, of necessity, return to this point.

G_3-Termination

A solution for the roots of Equation (82) has not been accomplished. Two considerations account for the difficulty involved in producing such a solution. The first, and the most obvious, arises from the fact that any macroscopic system of interest has $N_o \sim N^{23}$, thereby making the number of roots $\sim 10^{23}$. The second difficulty is found in the coupling of $\mathcal{G}_1(kt)$ to each of the $(N_o + 1)$-equations of motion. This is reflected in the determinant of Equation (82) by the presence of a nonzero member in each position of the first column. Except for these terms the equations of motion for $\mathcal{G}_j(kt)$ couples to $\mathcal{G}_{j-1}(kt)$ and $\mathcal{G}_{j+1}(kt)$ only. This difficulty is compounded by the presence of the fluctuation term Δ_j in the first member of the j^{th} row. For $j \geq 2$

$$\Delta_j = \langle (b_o^+)^{j-1} (b_o)^{j-1} \rangle = i G_j(\ell=0, t=\sigma)$$

$$= i \sum_k \mathcal{G}_j(k, t=\sigma) = \sum_k H_{jk} ,$$

where the H_{jk} are just the $N_o(N_o + 1)$ initial conditions mentioned earlier. But we have seen that a prior knowledge of these constants is not required for a solution as long as the ground state is the

averaging state. Thus, we expect that the solution for the $\mathcal{G}_j(kt)$, and consequently for the $G_j(\ell t)$, will be in terms of these Δ_j's, thereby requiring a self-consistent solution for these fluctuation terms.

As an alternative to the solution for the $(N_o+1)^2$ characteristic roots and the (N_o+1) Green's functions, we propose a decoupling of Equations (76), and hence Equations (80), by letting

$$G_3(\ell t) = \chi(x)\, G_1(\ell t), \tag{87}$$

where $\chi(x)$ is an undetermined function of the parameter x defined in Chapter II. This type of approximation is suggested by the Hartree-type approximations used in Chapter IV for $D_j(\ell t)$ and $E_j(\ell t)$. They are

$$D_j(\ell t) = -i \sum_{r'} \langle T[b_\ell^\dagger(t)]^{j-1}[b_\ell(t)]^{j-1} b_{\ell+r'}(t)\, b_o^\dagger(0)\rangle$$

$$\simeq -i \langle [b_\ell^\dagger(t)]^{j-1}[b_\ell(t)]^{j-1}\rangle \sum_{r'} \langle T\, b_{\ell+r'}(t)\, b_o^\dagger(0)\rangle = \Delta_j \sum_{r'} G_1(\ell+r', t)$$

$$E_j(\ell t) = -i \sum_{r'} \langle T\, b_{\ell+r'}^\dagger(t)\, [b_\ell^\dagger(t)]^{j-2}[b_\ell(t)]^{j} b_o^\dagger(0)\rangle$$

$$\simeq -i \sum_{r'} \langle b_{\ell+r'}^\dagger(t)\, b_\ell(t)\rangle \langle T[b_\ell^\dagger(t)]^{j-2}[b_\ell(t)]^{j-1} b_o^\dagger(0)\rangle \sim g_j\, G_{j-1}(\ell t).$$

A similar approximation for G_3 gives

$$G_3(\ell t) = -i \langle T\,[b_\ell^\dagger(t)]^2[b_\ell(t)]^3 b_o^\dagger(0)\rangle$$

$$\simeq -i \langle [b_\ell^\dagger(t)]^2[b_\ell(t)]^2\rangle \langle T\, b_\ell(t)\, b_o^\dagger(0)\rangle = \Delta_3 G_1(\ell t),$$

suggesting that χ of Equation (87) might be chosen as Δ_3.

A second suggestion for χ can be obtained by requiring that G_3 possess the correct discontinuity at $t = 0$. By Equation (77)

$$i\,G_3(\ell, t=0^+) - i\,G_3(\ell, t=0^-) \;=\; 3\,\Delta_3\,\delta_{\ell 0}\,,$$

whereas by Equation (77) and (87)

$$i\,G_3(\ell, t=0^+) - i\,G_3(\ell, t=0^-) = \chi\,[i\,G_1(\ell, t=0^+) - i\,G_1(\ell, t=0^-)]$$

$$= \chi\,\delta_{\ell 0}\,,$$

giving $3\Delta_3$ as the choice for χ.

Still another value for χ is suggested if we consider the value of G_3 at $\ell = 0$ and $t = 0^-$. By definition

$$i\,G_3(\ell=0, t=0^-) = \langle b_0^+ b_0^+ b_0^+ b_0 b_0 b_0 \rangle = \langle n_0(n_0-1)(n_0-2)\rangle = \Delta_4\,;$$

whereas by Equation (87)

$$i\,G_3(\ell=0, t=0^-) = \chi\,i\,G_1(\ell=0, t=0^-) \;=\; \chi\,,$$

suggesting that χ is best selected as Δ_4.

Gersch and Knollman (23) terminate these equations by letting $G_3 \equiv 0$, reasoning that this corresponds to limiting the ground state to cell occupancies ≤ 2. Let us consider this point. Suppose the ground state to be approximated by an optimum superposition of states diagonal in occupation-number space which satisfy the constraint that cell occupancies be zero, one, or two. Denote this state by $|2\rangle$ and use it as the averaging state in the $G_j(\ell t)$. Now

$$i\,G_3^-(\ell t) = \Theta(-t)\,\langle 2|\, b_0^+(0)\, b_\ell^+(t)\, b_\ell^+(t)\, b_\ell(t)\, b_\ell(t)\, b_\ell(t)\,|2\rangle$$

and

$$i\,G_3^+(\ell t) = \Theta(t)\,\langle 2|\, b_\ell^+(t)\, b_\ell^+(t)\, b_\ell(t)\, b_\ell(t)\, b_\ell(t)\, b_0^+(0)\,|2\rangle\,.$$

We see immediately that $G_3^- \equiv 0$ since $(b_\ell)^3$ operating on cells of occupancy of 0, 1, or 2 yields zero. Likewise, $G_3^+(\ell \neq 0, t) = 0$ for the same reason, while

$$i\, G_3^+(\ell=0,t) = \langle 2 | b_0^+(t)\, b_0^+(t)\, b_0(t)\, b_0(t)\, b_0(t)\, b_0^+(0) | 2 \rangle \neq 0 ,$$

so that

$$G_3(\ell t) = G_3^+(\ell, t)\, \delta_{\ell 0} ,$$

a slight deviation from $G_3 \equiv 0$.

Our approach in this G_3-termination shall be to use Equation (87) for G_3 and leave χ as an undetermined function of x. This freedom to specify χ will prove vital in obtaining the best possible solution for G_1 and G_2. We delay further discussion on this point until the following chapter where we solve the equations of motion, which are now

$$\left(\frac{i}{\rho u_0}\frac{\partial}{\partial t} - 3x + xS\right) \mathcal{G}_1(kt) - \mathcal{G}_2(kt) = 0 \qquad (88)$$

$$\left(2xS - \frac{x}{2}q_2 - \chi\right) \mathcal{G}_1(kt) + \left(\frac{i}{\rho u_0}\frac{\partial}{\partial t} - 3x - 1\right) \mathcal{G}_2(kt) = 0 . \qquad (89)$$

G_4-Termination

The G_3-termination proposed above is utilized in the next two chapters. In Chapter VI we obtain solutions for $\mathcal{G}_1(kt)$ and $\mathcal{G}_2(kt)$ and compare the results of this solution with a number of phenomena associated with the solid and liquid phases of He^4 at absolute zero. Recall that three distinct simplifications have been made in obtaining Equations (88) and (89):

(a) Starting with the problem of N_0 bosons interacting via a pair potential, we define a cell space and a corresponding cell model

Hamiltonian. Then the Green's functions, $G_j(\ell t)$, are defined and exact equations of motion obtained.

(b) The equations of motion for the G_j involve more complicated Green's functions which we label $D_j(\ell t)$ and $E_j(\ell t)$. These functions are approximated in terms of the G_j, resulting in $(N_o + 1)$ equations of motion involving the G_j functions and no others.

(c) The equations of motion of (b) are terminated by approximating G_3 in terms of G_1, and letting $G_j \equiv 0$ for $j > 3$.

With this number of approximations built into a calculation, any success it might demonstrate in reproducing observed phenomena is quite naturally suspect. While no unimpeachable arguments will be presented to substantiate any such predictions, we shall attempt to present consistency arguments as well as plausibility appeals. In this line we first consider the result of a terminating of the Green's functions' equations of motion by a G_4-termination, namely

$$G_4(\ell t) = \lambda\, G_1(\ell t)\,,$$

or correspondingly

$$\mathcal{G}_4(kt) = \lambda\, \mathcal{G}_1(kt),$$

where λ is an unspecified function of the parameter x.

From Equations (80) we see that such an approximation results in the following equations of motion:

$$\left(\frac{i}{\rho u_o}\frac{\partial}{\partial t} - 3x + xS\right)\mathcal{G}_1(kt) - \mathcal{G}_2(kt) = 0$$

$$(2xS - \tfrac{x}{2}q_2)\mathcal{G}_1(kt) + \left(\frac{i}{\rho u_o}\frac{\partial}{\partial t} - 3x - 1\right)\mathcal{G}_2(kt) - \mathcal{G}_3(kt) = 0$$

$$(3\Delta_3 x S - \lambda)\,\mathcal{G}_1(kt) - x q_3\,\mathcal{G}_2(kt) + \left(\frac{i}{\rho u_0}\frac{\partial}{\partial t} - 3x - 2\right)\mathcal{G}_3(kt) = 0.$$

Alternate Correction to the G_3-Termination

The G_4-termination just suggested could be used to substantiate any results of the earlier G_3-termination by demonstrating that such a termination does not change any important results appreciably. This presupposes that a higher order solution to the equations of motion obtained in Chapter IV (by approximating the D and E functions) represents a better solution. It is possible that the error introduced by the approximation of the D and E functions is comparable to that introduced in writing $\mathcal{G}_3$ as $\chi\,\mathcal{G}_1$. In such a case the G_4-termination attempts to improve the calculation by improving only one of two comparable approximations. An alternate procedure which attempts to improve both is now suggested.

Recall that the exact equation of motion for $G_2(\ell t)$ is

$$\left(\frac{i}{\rho u_0}\frac{\partial}{\partial t} - 3x - 1\right)G_2(\ell t) + x\,D_2(\ell t) - \tfrac{x}{2}\,E_2(\ell t) - G_3(\ell t) = 0 .$$

As a result of approximating D_2, E_2, and G_3 in terms of G_1, this equation becomes

$$\left(\frac{i}{\rho u_0}\frac{\partial}{\partial t} - 3x - 1\right)G_2(\ell t) - \left(\tfrac{x}{2}q_2 + \chi\right)G_1(\ell t) + x\sum_{r'} G_1(\ell + r'; t) = 0.$$

If we now define a function $U(\ell t)$ by

$$U(\ell t) = x\,D_2(\ell t) - \tfrac{x}{2}\,E_2(\ell t) - G_3(\ell t) + \left(\tfrac{x}{2}q_2 + \chi\right)G_1(\ell t) - x\sum_{r'} G_1(\ell + r'; t) = 0,$$

then the correct equation of motion for G_2 may be written

$$\left(\frac{i}{\rho u_0}\frac{\partial}{\partial t} - 3x - 1\right) G_2(\ell t) - \left(\frac{x}{2} g_2 + x\right) G_1(\ell t) + x \sum_{r'} G_1(\ell + r'; t) + U(\ell t) = 0.$$

This suggests that we might improve the calculations by obtaining an equation of motion for $U(\ell t)$ and use this equation in conjunction with those for G_1 and G_2 to obtain a more satisfactory solution.

CHAPTER VI

THE G_3-TERMINATION

The equations of motion for $\mathcal{G}_j(kt)$ obtained in the previous chapters (by a series of approximations leading to what we term the G_3-termination) are

$$\left[\frac{i}{\rho u_0}\frac{\partial}{\partial t} - 3\chi + \chi S(k)\right]\mathcal{G}_1(kt) - \mathcal{G}_2(kt) = 0 \tag{90}$$

$$\left[2\chi S(k) - \gamma(\chi)\right]\mathcal{G}_1(kt) + \left[\frac{i}{\rho u_0}\frac{\partial}{\partial t} - 3\chi - 1\right]\mathcal{G}_2(kt) = 0, \tag{91}$$

where we have defined the function γ by

$$\gamma(\chi) = \frac{\chi}{2} g_2(\chi) + \chi(\chi) . \tag{92}$$

Since $\chi(\chi)$ and $g_2(\chi)$ are, as yet, unspecified, we may consider $\gamma(\chi)$ to be a function which may be chosen as needed. We have shown that $\mathcal{G}_1$ and $\mathcal{G}_2$ obey the jump conditions

$$i\left[\mathcal{G}_1(k, t=0^+) - \mathcal{G}_1(k, t=0^-)\right] = 1 \tag{93}$$

$$i\left[\mathcal{G}_2(k, t=0^+) - \mathcal{G}_2(k, t=0^-)\right] = 2 . \tag{94}$$

Our objective in this chapter is to obtain solutions for $\mathcal{G}_1(kt)$ and $\mathcal{G}_2(kt)$ and from these solutions to extract any physical information which we can relate to He^4 at the absolute zero of temperature.

The characteristic equation for the coupled system of Equations (90) and (91) is obtained by letting

$$\mathcal{G}_1(kt) = a_1(k)\, e^{-i\omega t}$$

$$\mathcal{G}_2(kt) = a_2(k)\, e^{-i\omega t} ,$$

which gives, upon substitution into Equations (90) and (91),

$$(\nu - 3x + xS)\, a_1 \qquad - a_2 \qquad = 0$$

$$(2xS - \gamma)\, a_1 + (\nu - 3x - 1)\, a_2 = 0 ,$$

where

$$\nu = \frac{\omega}{\rho U_0} .$$

The determinant of coefficients yields the characteristic polynomial

$$\begin{vmatrix} \nu - 3x + xS & -1 \\ 2xS - \gamma & \nu - 3x - 1 \end{vmatrix} = (\nu - 3x)^2 - (1 - xS)(\nu - 3x) + xS - \gamma ,$$

whose two roots are

$$\nu_\pm(k) = 3x + \tfrac{1}{2}\left[1 - xS(k) \pm \sqrt{1 - 6xS(k) + x^2 S^2(k) + 4\gamma(x)}\right]$$

or

$$\omega_\pm(k) = 6K + \frac{\rho U_0}{2}\left[1 - xS(k) \pm \sqrt{1 - 6xS(k) + x^2 S^2(k) + 4\gamma(x)}\right] . \quad (95)$$

We note that the two roots are real if, and only if, the quantity under the square root is nonnegative, i.e.,

$$1 - 6xS + x^2 S^2 + 4\gamma(x) \geq 0 .$$

For the moment let us consider only the case where the roots are distinct, in which case

$$1-6\chi S+\chi^2 S^2+4\gamma>0 .$$

Since

$$S(k)=\sum_{i=1}^{3}\cos\frac{2\pi k_i}{2N+1} ,$$

it has an upper bound of $+3$ and a lower bound of -3, so that

$$-3 \leq S \leq 3 .$$

Note that the upper bound occurs for $k_1 = k_2 = k_3 = 0$, in which case $k = 0$. It follows, then, that

$$1-6\chi S+\chi^2 S^2+4\gamma \geq 1-18\chi+9\chi^2+4\gamma ,$$

with equality occurring for $k = 0$. Thus we obtain real, distinct characteristic values for Equations (90) and (91) for those values of χ such that

$$1-18\chi+9\chi^2+4\gamma>0 . \tag{96}$$

Normally we would use as a trial solution for $\mathcal{Y}_1$ and $\mathcal{Y}_2$

$$i\mathcal{Y}_1(kt) = a_1^+(k)e^{-i\omega_+ t} + a_1^-(k)e^{-i\omega_- t}$$

$$i\mathcal{Y}_2(kt) = a_2^+(k)e^{-i\omega_+ t} + a_2^-(k)e^{-i\omega_- t} ,$$

where the coefficients $a_j^{\pm}(k)$ are to be determined by appropriate initial conditions. In this case, however, two additional considerations must be included:

(a) We expect a solution for $t > 0$ and one for $t < 0$ which "fit" together at $t = 0$ according to the jump conditions of Equations (93) and (94).

(b) We have seen in Chapter III that the $t > 0$ solution must have no frequencies less than the maximum frequency of the $t < 0$ solution.

These two considerations require that $\omega_+(k)$ is to be associated with the $t > 0$ portion and $\omega_-(k)$ with the $t < 0$ portion. Therefore for a solution we try

$$i\mathcal{G}_1(kt) = a_1^+ \Theta(t)\, e^{-i\omega_+ t} + a_1^- \Theta(-t)\, e^{-i\omega_- t} \tag{97}$$

$$i\mathcal{G}_2(kt) = a_2^+ \Theta(t)\, e^{-i\omega_+ t} + a_2^- \Theta(-t)\, e^{-i\omega_- t}, \tag{98}$$

where

$$\Theta(t) \quad \left\{ \begin{array}{ll} 1 & \text{for } t>0 \\ 0 & \text{for } t<0 \end{array} \right\}.$$

Substitution of Equations (97) and (98) into Equation (90) for $t > 0$ and $t < 0$ gives

$$(\nu_+ - 3x + xS)a_1^+ - a_2^+ = 0 \tag{99}$$

$$(\nu_- - 3x + xS)a_1^- - a_2^- = 0,$$

while substitution into Equations (93) and (94) gives

$$a_1^+ - a_1^- = 1 \tag{100}$$

$$a_2^+ - a_2^- = 2.$$

From Equations (99) and (100) we see that

$$a_1^{\mp}(k) = \frac{1}{2}\left[\frac{3 - xS(k)}{\nu_+(k) - \nu_-(k)} \pm 1\right]$$

$$a_2^{\pm}(k) = \frac{1 - xS(k) + \gamma}{\nu_+(k) - \nu_-(k)} \pm 1 \quad ,$$

where

$$\nu_+(k) - \nu_-(k) = \sqrt{1 - 6xS(k) + x^2 S^2(k) + 4\gamma} \quad > 0.$$

Thus we have

$$i\mathcal{G}_1(kt) = \frac{\Theta(t)}{2}\left[\frac{3 - xS}{\nu_+ - \nu_-} + 1\right] e^{-i\omega_+ t} + \frac{\Theta(-t)}{2}\left[\frac{3 - xS}{\nu_+ - \nu_-} - 1\right] e^{-i\omega_- t} \tag{101}$$

$$i\mathcal{G}_2(kt) = \Theta(t)\left[\frac{1 - xS + \gamma}{\nu_+ - \nu_-} + 1\right] e^{-i\omega_+ t} + \Theta(-t)\left[\frac{1 - xS + \gamma}{\nu_+ - \nu_-} - 1\right] e^{-i\omega_- t} \tag{102}$$

as our solution for those values of x such that

$$1 - 18x + 9x^2 + 4\gamma(x) > 0.$$

We recover the spatial Green's functions by recalling that

$$G_j(lt) = \frac{1}{N_0} \sum_k \mathcal{G}_j(kt)\, e^{\frac{2\pi i\, k\cdot l}{2N+1}} \quad ,$$

so that

$$i G_1(lt) = \frac{\Theta(t)}{2N_0} \sum_k \left(\frac{3 - xS}{\nu_+ - \nu_-} + 1\right) e^{\frac{2\pi i k\cdot l}{2N+1} - i\omega_+ t} + \frac{\Theta(-t)}{2N_0} \sum_k \left(\frac{3 - xS}{\nu_+ - \nu_-} - 1\right) e^{\frac{2\pi i k\cdot l}{2N+1} - i\omega_- t} \tag{103}$$

$$i G_2(lt) = \frac{\Theta(t)}{N_0} \sum_k \left(\frac{1 - xS + \gamma}{\nu_+ - \nu_-} + 1\right) e^{\frac{2\pi i k\cdot l}{2N+1} - i\omega_+ t} + \frac{\Theta(-t)}{N_0} \sum_k \left(\frac{1 - xS + \gamma}{\nu_+ - \nu_-} - 1\right) e^{\frac{2\pi i k\cdot l}{2N+1} - i\omega_- t} . \tag{104}$$

Determination of $\gamma(x)$

In this cell model we require the cell size to vary with density in such a manner that the average number of particles per cell is exactly one, i.e.,

$$\langle m_0 \rangle = \langle b_0^+ b_0 \rangle = i G_1(l=0, t=0^-) = 1 \quad . \tag{105}$$

Substituting Equation (103) into Equation (105) yields

$$\frac{1}{2N_0}\sum_{k}\left[\frac{3-xS}{\nu_+-\nu_-}-1\right] = 1 ,$$

or

$$\frac{1}{N_0}\sum_{k}\frac{3-xS(k)}{\sqrt{1-6xS(k)+x^2S^2(k)+48\gamma(k)}} = 3. \qquad (106)$$

It is this condition that we use to evaluate the, as yet, undetermined function $\gamma(k)$.

Recall that

$$S(k) = \sum_{i=1}^{3}\cos\frac{2\pi k_i}{2N+1} ,$$

and that the sum over k indicated in Equation (106) is actually a triple sum over the three components k_1, k_2, k_3 of k, i.e.,

$$\sum_{k} = \sum_{k_1=-N}^{N}\sum_{k_2=-N}^{N}\sum_{k_3=-N}^{N} .$$

Let us define the quantities

$$\theta_i = \frac{2\pi k_i}{2N+1} , \qquad i = 1,2,3$$

so that a change in k_i of $+1$ corresponds to a change in θ_i of

$$\Delta\theta_i = \frac{2\pi}{2N+1}\Delta k_i = \frac{2\pi}{2N+1}$$

which is much less than one in this problem since $N \sim 10^{20}$. Recalling that

$$N_0 = (2N+1)^3 ,$$

we can write Equation (106) as

$$\sum_{k_1=-N}^{N}\sum_{k_2=-N}^{N}\sum_{k_3=-N}^{N} F\left(x, \frac{2\pi k_1}{2N+1}, \frac{2\pi k_2}{2N+1}, \frac{2\pi k_3}{2N+1}\right) \frac{1}{(2N+1)^3} = 3 ,$$

or

$$\frac{1}{(2\pi)^3} \sum_{\Theta_1}\sum_{\Theta_2}\sum_{\Theta_3} F(x, \Theta_1, \Theta_2, \Theta_3)\, \Delta\Theta_1\, \Delta\Theta_2\, \Delta\Theta_3 = 3 , \tag{107}$$

where

$$F(x, \Theta_1, \Theta_2, \Theta_3) = \frac{3 - x\sum_{i=1}^{3}\cos\Theta_i}{\sqrt{1 - 6x\sum_{i=1}^{3}\cos\Theta_i + x^2\left(\sum_{i=1}^{3}\cos\Theta_i\right)^2 + 4\gamma(x)}} .$$

Since $\Delta\theta_i \to 0$ as $N \to \infty$, and since $F(x, \theta_1, \theta_2, \theta_3)$ is a continuous function of θ_1, θ_2, and θ_3 in the region

$$-\pi \le \Theta_1, \Theta_2, \Theta_3 \le \pi ,$$

provided Equation (96) is satisfied, the triple sum of Equation (107) defines the triple integral

$$\frac{1}{(2\pi)^3} \int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} F(x, \Theta_1, \Theta_2, \Theta_3)\, d\Theta_1\, d\Theta_2\, d\Theta_3 = 3$$

as $N \to \infty$. F is an even function of θ_1, θ_2, and θ_3 so that

$$\frac{1}{\pi^3} \int_{0}^{\pi}\int_{0}^{\pi}\int_{0}^{\pi} F(x, \Theta_1, \Theta_2, \Theta_3)\, d\Theta_1\, d\Theta_2\, d\Theta_3 = 3 . \tag{108}$$

More convenient forms of Equation (108) are

$$\frac{1}{\pi^3} \int_R \frac{3 - xS}{\sqrt{1 - 6xS + x^2S^2 + 4\gamma}}\, d^3\Theta = 3 \tag{109}$$

and

$$\frac{1}{\pi^3} \int_R (3 - xS)\, f(x, S)\, d^3\Theta = 3 , \tag{110}$$

where

$$S = \sum_{i=1}^{3} \cos\Theta_i \quad ,$$

$$f(x,S) = \left[1 - 6xS + x^2S^2 + 4\gamma(x)\right]^{-1/2} ,$$

$$d^3\Theta = d\Theta_1\, d\Theta_2\, d\Theta_3 ,$$

and R denotes the region $0 \le \theta_1, \theta_2, \theta_3 \le \pi$.

We have, in principle, now evaluated $\gamma(x)$ by requiring that γ be that function of x which insures the exactness of Equation (109), while simultaneously satisfying the earlier requirement that

$$1 - 18x + 9x^2 + 4\gamma(x) > 0 .$$

In Appendix C we obtain a power series in x for f, substitute it into Equation (110), and obtain a power series for γ. The results to second power in x are

$$\gamma(x) = 9x^2 \tag{111}$$

$$f(x,S) = 1 + 3Sx + (13S^2 - 18)x^2 . \tag{112}$$

Ground State Energy and Fluctuation Terms

The expectation value for the ground state energy is

$$E = \langle H \rangle = \frac{\rho U_0}{2} \sum_{\ell} \langle b_\ell^+ b_\ell^+ b_\ell b_\ell \rangle + 6K \sum_{\ell} \langle b_\ell^+ b_\ell \rangle - K \sum_{\ell} \sum_{r'} \langle b_\ell^+ b_{\ell+r'} \rangle . \tag{113}$$

The translational symmetry of the cell model requires the average of a cell operator, say, $b_\ell^+ b_\ell^+ b_\ell b_\ell$, to be independent of the particular cell chosen so that

$$\sum_{\ell} \langle b_\ell^+ b_\ell^+ b_\ell b_\ell \rangle = N_0 \langle b_0^+ b_0^+ b_0 b_0 \rangle = N_0 \Delta(x) \quad ,$$

$$\sum_{\ell} \langle b_\ell^+ b_\ell \rangle = N_0 \langle b_0^+ b_0 \rangle = N_0$$

and

$$\sum_{\ell} \sum_{r'} \langle b_\ell^+ b_{\ell+r'} \rangle = N_0 \sum_{r'} \langle b_0^+ b_{r'} \rangle = N_0 h(x) \, .$$

Thus the ground state energy for the cell model as a function of the parameter x is

$$E = N_0 \left[\frac{\rho U_0}{2} \Delta(x) + 6K - K h(x) \right] \quad ,$$

or the energy per particle is

$$\varepsilon(x) = \frac{E}{N_0} = 6K \left[1 - \frac{1}{6} h(x) + \frac{1}{6x} \Delta(x) \right] \quad , \tag{114}$$

where both $h(x)$ and $\Delta(x)$ are fluctuation terms.

For the G_3-termination evaluation of $h(x)$ we get

$$h(x) = \sum_{r'} \langle b_0^+ b_{r'} \rangle = i \sum_{r'} G_1(\ell = 0, t = 0^-)$$

$$= \frac{i}{N_0} \sum_{k} \mathcal{Y}_1(k, t = 0^-) \sum_{r'} e^{\frac{2\pi i \, k \cdot r'}{2N+1}}$$

$$= \frac{2i}{N_0} \sum_{k} S(k) \, \mathcal{Y}_1(k, t = 0^-)$$

$$= \frac{1}{N_0} \sum_{k} S\left(\frac{3 - x S}{\nu_+ - \nu_-} - 1 \right) .$$

The triple sum over the k_i is converted into a triple integral as before:

$$h(x) = \sum_{k_1=-N}^{N} \sum_{k_2=-N}^{N} \sum_{k_3=-N}^{N} S(k) \left[\frac{3 - x S(k)}{\nu_+(k) - \nu_-(k)} - 1 \right] \frac{1}{(2N+1)^3}$$

$$= \frac{1}{(2\pi)^3} \sum_{\theta_1} \sum_{\theta_2} \sum_{\theta_3} S\left(\frac{3-xS}{\nu_+-\nu_-} - 1\right) \Delta\theta_1 \Delta\theta_2 \Delta\theta_3$$

$$\longrightarrow \frac{1}{(2\pi)^3} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} S\left(\frac{3-xS}{\nu_+-\nu_-} - 1\right) d^3\theta$$

But

$$\int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} S \; d^3\theta = 0 ,$$

and again the integrand is even in θ so that

$$h(x) = \frac{1}{\pi^3} \int_R \frac{(3-xS)S}{\nu_+-\nu_-} \, d^3\theta ,$$

or

$$h(x) = \frac{1}{\pi^3} \int_R (3-xS) S f(x,S) \, d^3\theta . \tag{115}$$

Similarly

$$\Delta(x) = \langle b_0^+ b_1^+ b_0 b_0 \rangle = i \, G_2(l=0, t=0^-)$$

$$= \frac{i}{N_0} \sum_k \mathcal{G}_2(k, t=0^-)$$

$$= \frac{1}{N_0} \sum_{k_1} \sum_{k_2} \sum_{k_3} \left(\frac{1-xS+\gamma}{\nu_+-\nu_-} - 1\right)$$

$$= \frac{1}{(2\pi)^3} \sum_{\theta_1} \sum_{\theta_2} \sum_{\theta_3} \left(\frac{1-xS+\gamma}{\nu_+-\nu_-} - 1\right) \Delta\theta_1 \Delta\theta_2 \Delta\theta_3$$

$$\longrightarrow \frac{1}{(2\pi)^3} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \left(\frac{1-xS+\gamma}{\nu_+-\nu_-} - 1\right) d^3\theta$$

$$= \frac{1}{\pi^3} \int_R \frac{1-xS+\gamma}{\nu_+-\nu_-} \, d^3\theta \; - 1 ,$$

or finally

$$\Delta(x) = \frac{1}{\pi^3} \int_R (1-xS+\gamma) f(x,S) \, d^3\theta \; - 1 . \tag{116}$$

In Appendix C the power series for $\gamma(x)$ and $f(x,s)$ given by Equations (111) and (112) are used to obtain the following lowest order expansions for $h(x)$ and $\Delta(x)$:

$$h(x) = 12x \tag{117}$$

$$\Delta(x) = 6x^2 \tag{118}$$

By Equation (114) the energy per particle is

$$\varepsilon(x) = 6K(1-x) \tag{119}$$

High Density Limit

In a physical system at very high densities the repulsive hard core interaction between particles is predominate over the attractive interaction which manifests itself at lower densities. The cell model can be expected to possess this same property if we require that the potential energy, ρU_o, resulting from a double cell occupancy be very large compared to the kinetic energy of localization, K, for high densities, i.e., the parameter

$$x = \frac{2K}{\rho U_o}$$

should approach zero in the high density limit. The effect of such a domination by the potential energy term is to produce a completely localized ground state. In this case the fluctuations are zero, and the ground state energy per particle is

$$\varepsilon = \frac{\langle H \rangle}{N_o} = \frac{\rho U_o}{2}\langle m_o(m_o-1)\rangle + 6K - K\sum_{r'}\langle b_o^+ b_{r'}\rangle = 6K,$$

just the energy required to localize the particle within the cell. The power series in x for $\varepsilon(x)$ is seen to agree with this argument since by Equation (119)

$$\lim_{x\to 0} \varepsilon(x) = 6K .$$

The fluctuation terms are also in agreement since by Equations (117) and (118),

$$\lim_{x\to 0} \Delta(x) = 0$$

$$\lim_{x\to 0} h(x) = 0 .$$

The solutions of the Green's functions obtained earlier in this chapter and the detailed knowledge of the nature of the ground state of the system as x approaches zero allows us to demonstrate in some detail the effect of the off-diagonal kinetic energy operator in the Hamiltonian as it lowers the system energy by moving particles.

Consider the cell model Hamiltonian

$$H = \frac{\rho U_o}{2} \sum_{\ell} m_\ell (m_\ell - 1) + 6K \sum_{\ell} m_\ell - K \sum_{\ell} \sum_{r} b_\ell^+ b_{\ell+r} .$$

If we, for the moment, neglect the last term, i.e., the off-diagonal kinetic energy operator, then H is diagonal in occupation number space. For a fixed number of particles the kinetic energy is now just $6K$ multiplied by the number of particles regardless of the distribution of particles in the cells. The potential energy has a minimum of zero and assumes this minimum when no cell occupancy exceeds unity. Thus the localized state corresponds to the ground state. For $(N_o - 1)$

particles the ground state for this modified Hamiltonian has the particles distributed one to a cell with one empty cell corresponding to an energy of $6K(N_o - 1)$. Similarly the N_o-particle ground state has one particle in each cell with an energy of $6KN_o$, while the $(N_o + 1)$-particle ground state has $(N_o - 1)$ singly occupied cells and one doubly-occupied cell with an energy of $\rho U_o + 6K(N_o + 1)$. Thus if we neglect the shift operator the $(N_o - 1)$- and N_o-particle ground states differ in energy by exactly $6K$ while the N_o- and $(N_o + 1)$-particle ground states differ by $\rho U_o + 6K$.

Let us now consider the effect of returning the shift operator to the Hamiltonian. We have stated in earlier chapters that we expect an energy lowering to result via increased particle wanderings. In the high density limit as x approaches zero, however, the potential energy domination negates particle wanderings by creation of a double and an empty from two singles. Thus any energy lowering must result from the "motion" of a double or a zero through the system. Since no doubles or zeroes exist in the N_o-particle ground state, such an effect should not be noticed. In the $(N_o - 1)$-particle ground state one empty cell exists, and we expect an energy lowering. Similarly the one double cell existing in the $(N_o + 1)$-particle system can move and cause an energy lowering. We now demonstrate these effects by appealing to the solutions for the Green's functions obtained in the first part of this chapter.

Recall that the minimum frequency associated with the $t > 0$ portion of the Green's functions corresponds to the difference in the

N_o and $(N_o + 1)$ ground state energies, i.e., the chemical potential μ^+. By Equation (95) the $t > 0$ frequencies are

$$\omega_+(k) = 6K + \frac{\rho U_o}{2}\left[1 - xS(k) + \sqrt{1 - 6xS(k) + x^2 S^2(k) + 4\gamma(x)}\right].$$

The minimum value of ω_+ occurs for $k = 0$, i.e., for $S = 3$, and so

$$\mu^+ = \omega_+(k=0) = 6K + \frac{\rho U_o}{2}\left[1 - 3x + \sqrt{1 - 18x + 9x^2 + 4\gamma(x)}\right].$$

Recalling that γ varies as x^2 for small x, we obtain for $x << 1$,

$$\mu^+ \simeq 6K + \rho U_o(1 - 6x). \tag{120}$$

Similarly the difference in the $(N_o - 1)$ and N_o ground state energies is

$$\mu^- = \omega_-(k=0) = 6K + \frac{\rho U_o}{2}\left[1 - 3x - \sqrt{1 - 18x + 9x^2 + 4\gamma(x)}\right],$$

which for $x << 1$ becomes

$$\mu^- \simeq 6K + 3x\rho U_o. \tag{121}$$

The results of Equations (120) and (121) are to be compared to

$$\mu^+ = 6K + \rho U_o$$

and

$$\mu^- = 6K,$$

which are the corresponding quantities when the shift term is ignored. Just as we had expected, the decreased value of μ^+ reflects a relative lowering of the $(N_o + 1)$-particle ground state energy via the motion of the doubly-occuplied cell. Likewise the increased value of μ^- indicates

a lowering of the $(N_o - 1)$ ground state energy through the motion of the empty cell.

The interpretation of Equations (120) and (121) by Gersch and Knollman (23) is from a slightly different viewpoint. In short, their argument is that the shift operator creates doubles and empties in the system. The addition of a particle to a particular cell in the N_o-particle system adds a localization energy $6K$ and a potential energy $\rho U_o P_1(x)$, where $P_1(x)$ is the probability that the particular cell is occupied by only one particle. In the same way, the removal of a particle from a particular cell in the N_o-particle ground state releases $6K$ units of localization energy and $\rho U_o P_2(x)$ units of potential energy, where $P_2(x)$ is the probability that the cell is doubly occupied. From Equations (120) and (121) we get

$$P_1(x) = 1 - 6x \tag{122}$$

$$P_2(x) = 3x . \tag{123}$$

Now the probability, $P_o(x)$, that a cell is unoccupied must be the same as for double occupancy since the creation of a double in the localized state necessitates the simultaneous production of an empty. Therefore

$$P_o(x) = 3x .$$

Since we have assumed only zero, one, and two occupancies, the probability for a single should be unity decreased by the sum of the probabilities for zero and double occupancies, i.e.,

$$P_1(x) = 1 - P_0(x) - P_2(x) = 1 - 6x \ ,$$

in agreement with Equation (122).

Momentum Considerations

In the continuum case the operator

$$\alpha_k = (2L)^{-3/2} \int \psi(r)\, e^{-\frac{2\pi i k \cdot r}{2L}}\, d\tau$$

is introduced and found to be an operator which destroys a particle from the system and simultaneously removes an amount of linear momentum of $hk/2L$ from the system. Similarly

$$\alpha_k^+ = (2L)^{-3/2} \int \psi^+(r)\, e^{\frac{2\pi i k \cdot r}{2L}}\, d\tau$$

creates a particle and an additional momentum of $hk/2L$ in the system on which it acts. The two operators obey the commutation rules

$$\left[\alpha_k, \alpha_{k'}^+\right] = \delta_{k,k'}$$

$$\left[\alpha_k, \alpha_{k'}\right] = \left[\alpha_k^+, \alpha_{k'}^+\right] = 0 \ ,$$

while the operator $a_k^+ a_k$ measures the number of particles of momentum $hk/2L$ within the state upon which it acts.

The corresponding cell model operators are constructed by Fourier analyzing the cell operators b_l and b_l^+. Let

$$a_k = (N_0)^{-1/2} \sum_l b_l\, e^{-\frac{2\pi i k \cdot l}{2N+1}}$$

and

$$a_k^+ = (N_0)^{-1/2} \sum_l b_l^+\, e^{\frac{2\pi i k \cdot l}{2N+1}} \ .$$

We see that

$$[a_k, a_{k'}^+] = \frac{1}{N_0} \sum_{\ell} \sum_{\ell'} [b_\ell, b_{\ell'}^+] e^{\frac{2\pi i (k'\cdot\ell' - k\cdot\ell)}{2N+1}}$$

But

$$[b_\ell, b_{\ell'}^+] = \delta_{\ell,\ell'}$$

so that

$$[a_k, a_{k'}^+] = \frac{1}{N_0} \sum_{\ell} e^{\frac{2\pi i (k'-k)\cdot\ell}{2N+1}} = \delta_{k,k'} .$$

Also

$$[a_k, a_{k'}] = \frac{1}{N_0} \sum_{\ell} \sum_{\ell'} [b_\ell, b_{\ell'}] e^{-\frac{2\pi i (k\cdot\ell + k'\cdot\ell')}{2N+1}} = 0 ,$$

since

$$[b_\ell, b_{\ell'}] = 0 ;$$

and

$$[a_k^+, a_{k'}^+] = \frac{1}{N_0} \sum_{\ell} \sum_{\ell'} [b_\ell^+, b_{\ell'}^+] e^{\frac{2\pi i (k\cdot\ell + k'\cdot\ell')}{2N+1}} = 0 ,$$

since

$$[b_\ell^+, b_{\ell'}^+] = 0.$$

Furthermore the number operator is

$$N = \sum_{\ell} b_\ell^+ b_\ell = \frac{1}{N_0} \sum_{k} \sum_{k'} a_k^+ a_{k'} \sum_{\ell} e^{\frac{2\pi i (k'-k)\cdot\ell}{2N+1}} = \sum_{k} a_k^+ a_k .$$

Thus we interpret $a_k (a_k^+)$ as an operator which removes (adds) a particle and decreases (increases) the momentum by $hk/2L$ upon acting on a given state. Likewise $a_k^+ a_k$ averaged over a state yields the number of particles with momentum $hk/2L$. In our system of units with $\hbar = 1$ the momentum associated with k is $\pi k/L$.

We now calculate the momentum distribution of particles in the ground state as predicted by the solutions from the G_3-termination. Now

$$\langle a_k^+ a_k \rangle = \frac{1}{N_0} \sum_{\ell} \sum_{\ell'} \langle b_\ell^+ b_{\ell'} \rangle e^{\frac{2\pi i k\cdot(\ell-\ell')}{2N+1}} ,$$

but translational symmetry assures us that

$$\langle b_\ell^+ b_{\ell'} \rangle = \langle b_0^+ b_{\ell'-\ell} \rangle = i G_1(\ell'-\ell, t=0^-) .$$

Therefore

$$\langle a_k^+ a_k \rangle = \frac{i}{N_0} \sum_{\ell} \sum_{\ell'} G_1(\ell'-\ell, t=0^-) e^{\frac{-2\pi i k\cdot(\ell'-\ell)}{2N+1}} , \qquad (124)$$

and the periodicity of the cell model reduces the double sum of Equation (124) to

$$\langle a_k^+ a_k \rangle = \frac{i}{N_0} \sum_{\ell} \sum_{\ell''} G_1(\ell'', t=0^-) e^{\frac{-2\pi i k\cdot\ell''}{2N+1}}$$

$$= i \sum_{\ell''} G_1(\ell'', t=0^-) e^{\frac{-2\pi i k\cdot\ell''}{2N+1}}$$

$$= i \mathcal{G}_1(k, t=0^-) .$$

With the G_3-termination, using Equation (101), we get

$$\langle a_k^+ a_k \rangle = \frac{1}{2}\left[\frac{3-xS(k)}{\sqrt{1-6xS(k)+x^2S^2(k)+4x}} - 1\right] . \qquad (125)$$

In the high density limit $x \to 0$, as does $\gamma(x)$, so that

$$\langle a_k^+ a_k \rangle \longrightarrow \frac{1}{2}\left[\frac{3}{1} - 1\right] = 1 ,$$

indicating a uniform momentum distribution, which reflects the localization of particles one to a cell.

A Critical Value of x Suggesting a Solid-Liquid Phase Change

The $(N_o + 1)$- and $(N_o - 1)$-particle states of momentum k differ in energy from the N_o-particle ground state by $\omega_+(k)$ and $\omega_-(k)$ respectively, where according to the G_3-termination,

$$\omega_\pm(k) = 6K + \frac{pU_o}{2}\left[1 - xS \pm \sqrt{1 - 6xS + x^2S^2 + 48}\right] . \qquad (126)$$

Now

$$S(k) = \cos\frac{2\pi k_1}{2N+1} + \cos\frac{2\pi k_2}{2N+1} + \cos\frac{2\pi k_3}{2N+1} ,$$

and therefore for small k

$$S \sim 3 - \tfrac{1}{2}\left(\frac{2\pi}{2N+1}\right)^2(k_1^2 + k_2^2 + k_3)^2 = 3 - \tfrac{1}{2}\left(\frac{2\pi k}{2N+1}\right)^2 .$$

But the momentum p associated with k is

$$p = \frac{\pi k}{L} = \frac{2\pi k}{(2N+1)\tau^{1/3}} = \frac{2\pi k}{2N+1}\rho^{1/3} ,$$

so that

$$\frac{2\pi k}{2N+1} = \rho^{-1/3} p ;$$

and therefore

$$S \sim 3 - \tfrac{1}{2}\rho^{-2/3}p^2 .$$

Thus for small momentum

$$\omega_\pm(p) = 6K + \frac{pU_o}{2}\left[1 - 3x + \tfrac{1}{2}x\rho^{-2/3}p^2 \pm \sqrt{1 - 18x + 9x^2 + 48 + 3(1-x)x\rho^{-2/3}p^2}\right] . \qquad (127)$$

We see that for low momentum excitations the excitation energy depends quadratically upon p, provided the quantity

$$1 - 18x + 9x^2 + 4\gamma(x)$$

appearing in the square root is greater than zero. This, however, is exactly the requirement for the solutions of the Green's functions obtained thus far to be correct. As mentioned earlier this quadratic momentum dependence of the single particle excitation is characteristic of solids.

We have also seen that the chemical potential which corresponds to the addition of a particle is

$$\mu^+ = \omega_+(0) = 6K + \frac{pU_0}{2}\left[1 - 3x + \sqrt{1 - 18x + 9x^2 + 4\gamma}\right], \quad (128)$$

while that corresponding to the removal of a particle is

$$\mu^- = \omega_-(0) = 6K + \frac{pU_0}{2}\left[1 - 3x - \sqrt{1 - 18x + 9x^2 + 4\gamma}\right]. \quad (129)$$

Thus the energy for adding a particle is greater than that for removing a particle by

$$\mu^+ - \mu^- = pU_0\sqrt{1 - 18x + 9x^2 + 4\gamma(x)} > 0, \quad (130)$$

a result which is again characteristic of a solid.

Inspection of Equations (127) and (130) suggests that if the quantity $1 - 18x + 9x^2 + 4\gamma(x)$ vanishes for some value of x, say x_0, then (a) the single particle excitation becomes linear for small momentum, and (b) the energies related to particle addition and particle removal become equal.

The equality of the energies for particle addition and particle removal is suggestive of a change to the liquid state as we argued in Chapter III. Furthermore, and perhaps more significantly, the linear momentum dependence of the excitation energy seems to correspond to the phonon portion of the Landau dispersion prediction for the He^4 superfluid discussed in Chapter I.

The momentum distribution also exhibits an interesting feature for $x = x_o$. From Equations (125) the occupation of the momentum state p is given by

$$\langle a_p^+ a_p \rangle = \frac{1}{2}\left[\frac{3 - xS}{\sqrt{1 - 6xS + x^2S^2 + 48}} - 1\right],$$

which for small momentum becomes

$$\langle a_p^+ a_p \rangle \simeq \frac{1}{2}\left[\frac{3(1-x) + \frac{1}{2}x\rho^{-2/3}\rho^2}{\sqrt{1 - 18x + 9x^2 + 48\gamma(x) + 3x(1-x)\rho^{-2/3}\rho^2}} - 1\right]. \qquad (131)$$

Assuming, for the moment, the existence of a value x_o such that

$$1 - 18x_o + 9x_o^2 + 48\gamma(x_o) = 0, \qquad (132)$$

we see that for small p

$$\langle a_p^+ a_p \rangle \sim \frac{1}{\rho},$$

indicating a high population of the low momentum states. This suggests the possibility of a finite fraction of the particles in the zero momentum state, i.e., a condensation of particles in momentum space, in analogy with the Bose-Einstein condensation for a gas of noninteracting bosons.

The discussion of the past few paragraphs hinges on the existence of a value $x_o > 0$ such that Equation (132) is satisfied. Since $\gamma(k)$ is determined from the normalization condition

$$\frac{1}{\pi^3}\int_R \frac{3-xs}{\sqrt{1-6xs+x^2s^2+4\gamma(x)}}\,d^3\theta = 3,$$

or, rearranging terms,

$$\frac{1}{\pi^3}\int_R \frac{3-xs}{\sqrt{1-18x+9x^2+4\gamma(x)+6x(3-s)-x^2(9-s^2)}}\,d^3\theta = 3,$$

the question resolves itself into asking if an $x_o > 0$ exists such that

$$\frac{1}{\pi^3}\int_R \frac{3-x_o s}{\sqrt{x_o(3-s)(6-3x_o-x_o s)}}\,d^3\theta = 3. \qquad (133)$$

In Appendix D we demonstrate that such an x_o exists and estimate its value to be 0.065 by an approximate evaluation of the integral of Equation (133). A second procedure for estimating x_o is to use the expansion of Equation (111) for γ to get

$$1 - 18x_o + 9x_o^2 + 4(9x_o^2) = 0$$

$$1 - 18x_o + 45x_o^2 = 0.$$

The roots of this quadratic equation are $1/15$ and $1/3$, the smaller root being the one we seek. Thus

$$x_o \sim \frac{1}{15} \simeq 0.067$$

is in good agreement with the previous estimate.

We now return to the Green's functions obtained for $0 \leq x < x_o$ and seek solutions for $x \geq x_o$.

Green's Functions and Related Quantities for $x \geq x_o$

The Green's functions obtained earlier in this chapter, namely,

$$i\mathcal{G}_1(kt) = \frac{\Theta(t)}{2}\left[\frac{3-xS}{\nu_+-\nu_-}+1\right]e^{-i\omega_+ t} + \frac{\Theta(-t)}{2}\left[\frac{3-xS}{\nu_+-\nu_-}-1\right]e^{-i\omega_- t}$$

$$i\mathcal{G}_2(kt) = \Theta(t)\left[\frac{1-xS+\gamma}{\nu_+-\nu_-}+1\right]e^{-i\omega_+ t} + \Theta(-t)\left[\frac{3-xS}{\nu_+-\nu_-}-1\right]e^{-i\omega_- t}$$

are valid for all k over the range $0 \leq x < x_o$. At $x = x_o$ the $k = 0$ solution fails, since for this value of x

$$\nu_+(0) = \nu_-(0) ,$$

and the solutions are not defined. Recall that

$$\mu^{\pm} = \omega_{\pm}(k=0) = \rho U_o \nu_{\pm}(k=0) ,$$

so that

$$\mu^+(x_o) = \mu^-(x_o) .$$

In Chapter III we argued that such a condition characterizes a liquid with the provision that μ^+ actually exceeds μ^- by a term of order $1/N_o$. Consequently let us require

$$\mu^+(x_o) = \mu^-(x_o) + \rho U_o \eta(x_o) , \tag{134}$$

where $\eta(x_o)$ is to be a quantity of order $1/N_o$. We have shifted the $\omega_+(k)$ curve by $\rho U_o \eta(x_o)$ so that

$$\omega_+(k) = 6K + \frac{pU_0}{2}\left[1 - x_0 S + \sqrt{x_0(3-S)(6-3x_0-x_0S)}\,\right] + pU_0\eta(x_0)$$

while

$$\omega_-(k) = 6K + \frac{pU_0}{2}\left[1 - x_0 S - \sqrt{x_0(3-S)(6-3x_0-x_0S)}\,\right].$$

With this provision for an infinitisimal difference in μ^+ and μ^-, the Green's functions are now defined for all k at x_0. We have

$$i\mathcal{G}_1(kt) = \frac{\Theta(t)}{2}\left[\frac{3-x_0S}{\sqrt{}+\eta_0}+1\right]e^{-i\omega_+ t} + \frac{\Theta(-t)}{2}\left[\frac{3-x_0S}{\sqrt{}+\eta_0}-1\right]e^{-i\omega_- t}$$

$$i\mathcal{G}_2(kt) = \Theta(t)\left[\frac{1-x_0S+\gamma}{\sqrt{}+\eta_0}+1\right]e^{-i\omega_+ t} + \Theta(-t)\left[\frac{1-x_0S+\gamma}{\sqrt{}+\eta_0}-1\right]e^{-i\omega_- t},$$

where

$$\sqrt{} = \sqrt{x_0(3-S)(6-3x_0-x_0S)}$$

and

$$\eta_0 = \eta(x_0).$$

Thus the momentum occupation is now

$$\langle a_p^+ a_p\rangle = i\mathcal{G}_1(p, t=0^-) = \frac{1}{2}\left[\frac{3-x_0S}{\sqrt{}+\eta_0}-1\right];$$

and in particular the zero momentum occupation is

$$\langle a_0^+ a_0\rangle = \frac{1}{2}\left[\frac{3(1-x_0)}{\eta_0}-1\right],$$

with fractional occupation

$$F_0 = \frac{\langle a_0^+ a_0\rangle}{N_0} = \frac{1}{2}\,\frac{3(1-x_0)}{N_0\eta_0} - \frac{1}{2N_0} \simeq \frac{3(1-x_0)}{N\eta_0}.$$

The exact dependence of η_o upon N_o is vital in determining the fractional occupation of the zero momentum state as the number of particles, N_o, approaches infinity. Suppose, for instance,

$$\eta_o = K/N_o \quad ,$$

then

$$F_o = \frac{3(1-x_o)}{2K}$$

is finite as $N_o \to \infty$; whereas if

$$\eta_o = K/N_o^{1-\varepsilon} \quad ,$$

then

$$F_o = \frac{3(1-x_o)}{K N_o^{\varepsilon}}$$

approaches zero as $N_o \to \infty$. To determine F_o at x_o, we use particle normalization allowing for a finite population of the zero momentum state, i.e.,

$$1 = \frac{1}{N_o}\sum_k \langle a_k^+ a_k \rangle = F_o + \frac{1}{N_o}\sum_{k\neq 0} \langle a_k^+ a_k \rangle$$

$$= F_o + \frac{1}{2\pi^3}\int_R \left[\frac{3-x_o S}{\sqrt{\quad + \eta_o}} - 1\right] d^3\Theta \, .$$

The integral on the righthand side of this equation (with $\eta_o = 0$) is just the particle normalization used to determine x_o as in Equation (133). Now the integral replacement for the sum is valid only for $N_o \to \infty$, in which case we require η_o to approach zero, so that this integral is unity, indicating that F_o is zero at the critical value of x, i.e., for $x = x_o$ the zero momentum state does not possess a finite occupation.

We now extend the Green's functions past x_o by utilizing the function $\gamma(x)$ appearing in the solution. Recall that

$$\omega_{\pm}(k) = 6K + \frac{pU_o}{2}\left[1 - xS \pm \sqrt{1 - 18x + 9x^2 + 4\gamma(x) + x(3-S)(6-3x-xS)}\right]$$

for $0 \leq x \leq x_o$. Over this range of x these frequencies are real since

$$1 - 18x + 9x^2 + 4\gamma(x) \geq 0$$

with equality occurring at x_o only. To keep the frequencies real for $x > x_o$ requires that $\gamma(x)$ be such that either

$$1 - 18x + 9x^2 + 4\gamma(x) = 0 \tag{135}$$

or

$$1 - 18x + 9x^2 + 4\gamma(x) > 0 \ . \tag{136}$$

We shall show that if γ is chosen to satisfy Equation (135), then solutions for the Green's functions follow which satisfy the cell model requirement of an average of one particle per cell, while if γ is chosen according to Equation (136), it is impossible to satisfy this normalization requirement.

Now let γ be such that Equation (135) is satisfied for $x_o \leq x \leq 1$. The upper bound on x is necessary to keep the $6 - 3x - xS$ term positive for all momentum. We note that this choice of $\gamma(x)$ also keeps the low momentum dependence of $\omega_{\pm}(k)$ linear and therefore retains the phonon character over these values of x.

To insure that the Green's functions be defined for all k on the range $x_o < x < 1$, we again shift the $t > 0$ frequencies by an

amount $\rho U_0 \eta(x)$, where we expect

$$\eta(x) \sim \Theta(1/N_0) .$$

Thus, just as at $x = x_0$, we have for $x_0 \le x < 1$,

$$i\mathcal{G}_1(kt) = \frac{\theta(t)}{2}\left[\frac{3-xs}{\sqrt{\quad}+\eta}+1\right]e^{-i\omega_+ t} + \frac{\theta(-t)}{2}\left[\frac{3-xs}{\sqrt{\quad}+\eta}-1\right]e^{-i\omega_- t}$$

$$i\mathcal{G}_2(kt) = \theta(t)\left[\frac{1-xs+\gamma}{\sqrt{\quad}+\eta}+1\right]e^{-i\omega_+ t} + \theta(-t)\left[\frac{1-xs+\gamma}{\sqrt{\quad}+\eta}-1\right]e^{-i\omega_- t} ,$$

where

$$\sqrt{\quad} = \sqrt{x(3-s)(6-3x-xs)} .$$

The momentum distribution is

$$\langle a_k^+ a_k \rangle = \frac{1}{2}\left[\frac{3-xs}{\sqrt{\quad}+\eta}-1\right] ,$$

with the zero momentum being given by

$$\langle a_0^+ a_0 \rangle = \frac{1}{2}\left[\frac{3(1-x)}{\eta}-1\right] .$$

Particle normalization requires

$$1 = F_0(x) + \frac{1}{2\pi^3}\int_R \left[\frac{3-xs}{\sqrt{\quad}+\eta}-1\right] d^3\theta ,$$

or letting $\eta \to 0$ in the integral

$$F_0(x) = \frac{1}{2}\left[3 - \frac{1}{\pi^3}\int_R \frac{3-xs}{\sqrt{x(3-s)(6-3x-xs)}}\, d^3\theta\right] . \qquad (137)$$

Consider the integral

$$I(x) = \frac{1}{\pi^3}\int_R \frac{3-xs}{\sqrt{x(3-s)(6-3x-xs)}}\, d^3\theta \qquad (138)$$

appearing in Equation (137). By Equation (133) we have

$$I(x_0) = 3 \ ,$$

so that, as we have seen

$$F_0(x_0) = \tfrac{1}{2}[3 - I(x_0)] = 0 \ .$$

Now for $x = 1$

$$I(1) = \frac{1}{\pi^3}\int \frac{3-S}{\sqrt{(3-S)(3-S)}}\, d^3\Theta = 1 \ ;$$

and thus

$$F_0(1) = \tfrac{1}{2}[3 - I(1)] = 1 \ ,$$

that is, all the particles have condensed to the zero momentum state.

The function $I(x)$ is differentiable on $x_0 < x < 1$ with derivative

$$\frac{dI}{dx} = -\frac{9(1-x)}{\pi^3}\int \frac{d^3\Theta}{\sqrt{x^3(3-S)(6-3x-xS)^3}} \left\{ \begin{array}{ll} < 0 & \text{for } x_0 < x < 1 \\ = 0 & \text{for } x = 1 \end{array} \right\} .$$

We conclude that $I(x)$ is a monotonically decreasing function on $x_0 < x < 1$ with bounds

$$3 > I(x) > 1 \ . \tag{139}$$

Since

$$F_0(x) = \tfrac{1}{2}[3 - I(x)] \ , \tag{140}$$

the occupation of the zero momentum state increases monotonically from zero to one as x increases from x_0 to unity.

The arguments leading to the macroscopic occupation of the zero momentum state as expressed by Equations (139) and (140) follow if we choose $\gamma(k)$ as in Equation (135). Solutions for the Green's functions also exist if γ is selected to satisfy the inequality of Equation (136). We can, however, demonstrate that such a choice of γ is not acceptable for this calculation in the following way. If Equation (136) is satisfied, $\mu^+ > \mu^-$, and Equations (101) and (102) are solutions of the Green's functions differential equations. The momentum occupation is given by

$$\langle a_p^+ a_p \rangle = i\mathcal{G}_1(p, t=0^-)$$
$$= \frac{1}{2}\left[\frac{3-xS}{\sqrt{1-18x+9x^2+4\gamma(x)+x(3-S)(6-3x-xS)}} - 1\right].$$

In particular the zero momentum occupation is

$$\langle a_0^+ a_0 \rangle = \frac{1}{2}\left[\frac{3(1-x)}{\sqrt{1-18x+9x^2+4\gamma(x)}} - 1\right],$$

with no indication of a macroscopic occupation. Particle normalization is given

$$1 = \frac{1}{2}\left[\frac{1}{\pi^3}\int \frac{3-xS}{\sqrt{1-18x+9x^2+4\gamma(x)+x(3-S)(6-3x-xS)}} d^3\Theta - 1\right].$$

Now for

$$1-18x+9x^2+4\gamma(x) > 0,$$

we get

$$\frac{1}{\pi^3}\int \frac{3-xS}{\sqrt{1-18x+9x^2+4\gamma(x)+x(3-S)(6-3x-xS)}} d^3\Theta < \frac{1}{\pi^3}\int \frac{3-xS}{\sqrt{x(3-S)(6-3x-xS)}} d^3\Theta$$
$$= I(x),$$

where $I(x)$ is defined by Equation (138). But for $x_o < x < 1$ we have from Equation (139) that

$$I(x) < 3 ,$$

in which case

$$\frac{1}{2}\left[\frac{1}{\pi^3}\int \frac{3-xS}{\sqrt{1-18x+9x^2+4\gamma(x)+x(3-x)(6-3x-xS)}}\, d^3\Theta - 1\right] < 1 .$$

Consequently this choice of γ does not permit us to satisfy the model requirement of one particle per cell.

Let us summarize the procedure which has evolved for determining γ. In both the solid region $(0 \leq x < x_o)$ and the superfluid region $(x_o < x)$, γ is determined by requiring that the average number of particles per cell is exactly one. As a result, for $0 \leq x < x_o$, γ is determined from the integral equation

$$\frac{1}{\pi^3}\int \frac{3-xS}{\sqrt{1-18x+9x^2+4\gamma(x)+x(3-S)(6-3x-xS)}}\, d^3\Theta = 3 ;$$

while for $x_o \leq x \leq 1$, γ is given by

$$\gamma(x) = 18x - 1 - 9x^2 .$$

Higher values for x need not be considered here since, as we shall see, experimental data indicates that the melting (25 atmospheres) to zero pressure region corresponds to a change in x of approximately twenty-five per cent. Since we have found the value of x_o to be about 0.065, the physically-meaningful range of x-values is apparently from x_o to approximately 0.1.

We may estimate the maximum occupation of the zero momentum state

in He^4 by use of Equation (140) and measured molar volumes at absolute zero. For x near x_0 and therefore $\ll 1$, the x dependence of

$$I(x) = \frac{1}{\sqrt{x}} \frac{1}{\pi^3} \int \frac{3 - xS}{\sqrt{(3-S)(6-3x-xS)}} d^3\theta$$

is predominately from the $1/\sqrt{x}$ term, since the other x terms combine additively with much larger quantities. Therefore

$$I(x) \simeq \frac{1}{\sqrt{x}} \frac{1}{\pi^3} \int \frac{3 - x_0 S}{\sqrt{(3-S)(6-3x_0-x_0S)}} d^3\theta = \sqrt{\frac{x_0}{x}}\, I(x_0) = 3\sqrt{\frac{x_0}{x}} ,$$

and so for x near x_0

$$F_0(x) \simeq \frac{3}{2}\left[1 - \sqrt{\frac{x_0}{x}}\right] .$$

Now

$$x = \frac{2K}{\rho u_0} = \frac{2 p^{2/3}}{2m\rho u_0} = \frac{1}{m u_0 \tau^{1/3}} ,$$

where τ is the volume per particle. If we assume the strength U_0 to be relatively insensitive to changes in τ, then

$$\frac{x_0}{x} \simeq \left(\frac{\tau_0}{\tau}\right)^{1/3}$$

and

$$F_0(\tau) \simeq \frac{3}{2}\left[1 - \left(\frac{\tau_0}{\tau}\right)^{1/6}\right] .$$

The molar volume of the solid at the melting pressure is about 21 cm^3, and at zero pressure it is about 28 cm^3. Thus at zero pressure we estimate

$$F_0 \simeq \frac{3}{2}\left[1 - \left(\frac{3}{4}\right)^{1/6}\right] \simeq 0.07 ,$$

i.e., a seven per cent occupation of the zero momentum state . This is in surprising agreement with an estimate of eight per cent obtained by Penrose and Onsager (22) in an extension of the Bose-Einstein condensation of the ideal gas to interacting particles.

CHAPTER VII

CONCLUSIONS

Although considerable effort has been expended over the past few decades in attempting to develop a satisfactory model for the superfluid phase of liquid helium, many problems remain unsolved. London's association of the λ-transition in helium with the Bose-Einstein condensation of an ideal Bose gas suggests that the superfluid is characterized by a macroscopic occupation of the zero momentum state. Attempts to treat the superfluid by considering bosons at low densities with repulsive interactions have assumed this macroscopic occupation from the outset. No convincing theoretical arguments have been presented which demonstrate how such a macroscopic occupation comes about without having to assume it.

Landau's explanation of superfluid properties in terms of assumed energy-momentum relations between the elementary excitations is very successful in predicting a number of observed phenomena, as mentioned in Chapter I. Unfortunately the justification of the full excitation spectrum from a system Hamiltonian has never been accomplished.

These remarks point out at least two of the questions which remain to be answered for the helium superfluid. First, can one demonstrate a macroscopic occupation of the zero momentum state for this phase of helium? Next, can one, starting with a system Hamiltonian, obtain Landau's excitation spectrum? In this study we have obtained affirmative answers to both of these questions.

The cell model used in this work represents an effort to avoid many of the difficulties experienced in approaching the superfluid phase from the low density region. By allowing the cell size to vary with density so that the number of cells remains equal to the number of particles, the model simulates a solid at high densities by localizing the particles one to a cell. This localization is caused by a prohibitively large potential energy requirement for placing two particles in the same cell. As the density decreases the off-diagonal kinetic energy operator in the Hamiltonian produces an energy lowering by allowing particles to stray from cell to cell, thus increasing the fluctuations and diminishing the extreme localization property of a solid. Using Green's functions we show, after a careful discussion of the approximations involved, that at a certain critical value of x (the ratio of the kinetic energy required to localize a particle to a cell to the additional potential energy required to add a second particle to a cell) the solutions exhibit three new properties which suggest the change from the solid phase to the superfluid phase:

(1) The energy for adding a particle to the system without creating excitations becomes equal to that for removing a particle. As indicated in Chapter III, this signals the beginning of a fluid phase.

(2) At this critical value of x the excitation spectrum changes from quadratic to linear for low momentum excitations. This phonon character for low momentum excitations is precisely the system property which accounts for superfluidity in Landau's phenomenological model for liquid helium.

(3) The two properties mentioned above are shown to be true for values of x greater than the critical value and therefore for densities less than the corresponding critical density. In addition the zero momentum state exhibits a macroscopic occupation for densities less than the critical density, while for densities greater than this critical value, a macroscopic occupation does not exist. We estimate the maximum occupation to be seven per cent. These results for a macroscopic occupation are particularly interesting since they represent a demonstration of this phenomenon starting from a system of interacting particles.

In this work there is no direct association of the results with He^4. That is, we have made no assumptions that uniquely identify these calculations with a particular isotope of a particular element. Arguments reviewed in Chapter I indicate that He^4 remains a liquid as the temperature approaches absolute zero because of its relatively small mass and weak attractive interaction. He^3, with an even smaller mass and similar interaction, also exhibits the liquid state at exceedingly low temperatures, but has shown no superfluidity.

On the basis of the preceding paragraph two questions seem to be particularly pertinent for future investigation. First, will the addition of sufficiently strong attractive interactions to the cell model Hamiltonian prohibit a solid-superfluid transition? Second, will the introduction of Fermi-Dirac statistics into the model remove the superfluid properties? An affirmative answer to each of these questions would supply considerable support to our proposal that the results contained here should rightfully be associated with the solid-superfluid transition in

He^4 at an absolute temperature of zero. J. Fernandez is currently considering both of these questions and has indicated by personal communication that the addition of sufficiently strong attractive interactions does remove the transition. Just what effect the change in statistics will have has not yet been determined.

Finally, there remains for possible future investigation, the detailed calculation of the effect of the higher order terminations which have been suggested in Chapter V. Of course, the complexity increases with each successively higher termination of the coupled equations. What one would probably desire then, is an indication of the qualitative effect that the higher order terminations have on the transition.

A P P E N D I C E S

APPENDIX A

DERIVATION OF EQUATION (22)

The operator $F_{\ell,j}$ is defined in Equation (21) as

$$F_{\ell,j} = [b_\ell^+]^{j-1} [b_\ell]^{j-1} . \tag{A1}$$

We wish to demonstrate that

$$F_{\ell,j} = \left\{ \begin{array}{ll} 1 & j=1 \\ n_\ell(n_\ell-1)\cdots(n_\ell-j+2) & j\geq 2 \end{array} \right\}, \tag{A2}$$

where

$$n_\ell = b_\ell^+ b_\ell .$$

Equation (A2) checks immediately for $j = 1$, since

$$F_{\ell,1} = (b_\ell^+)^0 (b_\ell)^0 = 1 .$$

We will demonstrate the validity (A2) by induction. For $j = 2$

$$F_{\ell,2} = [b_\ell^+] [b_\ell] = b_\ell^+ b_\ell = n_{\ell,1}$$

as required by Equation (A2). Now assume Equation (A2) to be true for $j = m > 1$, that is,

$$F_{\ell,m} = n_\ell(n_\ell-1)\cdots(n_\ell-m+2).$$

For $j = m+1$, we have

$$F_{\ell,m+1} = [b_\ell^+]^m [b_\ell]^m$$

$$= b_\ell^+ b_\ell \left[b_\ell^+\right]^{m-1} \left[b_\ell\right]^{m-1} - (m-1)\left[b_\ell^+\right]^{m-1}\left[b_\ell\right]^{m-1} ,$$

where we have applied the commutation relation

$$b_\ell b_\ell^+ - b_\ell^+ b_\ell = 1$$

$(m-1)$ times. We now have

$$F_{\ell,m+1} = (b_\ell^+ b_\ell - m+1)\left[b_\ell^+\right]^{m-1}\left[b_\ell\right]^{m-1}$$

$$= (n_\ell - m+1)\ F_{\ell,m}$$

$$= (n_\ell - m+1)\, n_\ell (n_\ell - 1)\cdots(n_\ell - m+2)$$

$$= n_\ell (n_\ell - 1)\cdots(n_\ell - m+2)(n_\ell - m+1) ,$$

which is the desired result.

APPENDIX B

DERIVATION OF EQUATION (53)

We wish to show that for $j \geq 1$

$$[F_{\ell,j}\, b_\ell, H] = \left\{ \begin{array}{l} [6K + (j-1)\rho U_0]\, F_{\ell,j}\, b_\ell \quad + \quad \rho U_0\, F_{\ell,j+1}\, b_\ell \\ \\ -jK \sum_{r'} F_{\ell,j}\, b_{\ell+r'} \quad + (j-1)K \sum_{r'} b^+_{\ell+r'} F_{\ell,j-1}\, b_\ell\, b_\ell \end{array} \right\}, \tag{B1}$$

where

$$F_{\ell,j} = (b^+_\ell)^{j-1} (b_\ell)^{j-1}$$

and

$$H = \frac{\rho U_0}{2} \sum_\ell b^+_\ell b^+_\ell b_\ell b_\ell + 6K \sum_\ell b^+_\ell b_\ell - K \sum_\ell \sum_{r'} b^+_\ell b_{\ell+r'} .$$

For $j = 1$

$$F_{\ell,1} = 1,$$

and so

$$[F_{\ell,1}\, b_\ell, H] = [b_\ell, H] \tag{B2}$$

$$= \frac{\rho U_0}{2} \sum_m [b_\ell, b^+_m b^+_m b_m b_m] + 6K \sum_m [b_\ell, b^+_m b_m] - K \sum_m \sum_{r'} [b_\ell, b^+_m b_{m+r'}].$$

Now

$$[b_\ell, b^+_m b^+_m b_m b_m] = b_\ell b^+_m b^+_m b_m b_m - b^+_m b^+_m b_m b_m b_\ell$$

$$= b^+_m b_\ell b^+_m b_m b_m + [b_\ell, b^+_m]\, b^+_m b_m b_m - b^+_m b^+_m b_m b_m b_\ell$$

$$= b^+_m [b_\ell, b^+_m] b_m b_m + [b_\ell, b^+_m]\, b^+_m b_m b_m$$

$$= 2 b_m^+ b_m b_m \delta_{\ell,m} ,$$

where we have used the commutation relations

$$[b_\ell, b_m^+] = \delta_{\ell,m}$$

$$[b_\ell, b_m] = 0 .$$

Also

$$[b_\ell, b_m^+ b_m] = b_\ell b_m^+ b_m - b_m^+ b_m b_\ell$$

$$= [b_\ell, b_m^+] b_m$$

$$= b_m \delta_{\ell,m} ,$$

and

$$[b_\ell, b_m^+ b_{m+r'}] = b_\ell b_m^+ b_{m+r'} - b_m^+ b_{m+r'} b_\ell$$

$$= [b_\ell, b_m^+] b_{m+r'}$$

$$= b_{m+r'} \delta_{\ell,m} .$$

Thus

$$[b_\ell, H] = pU_0 b_\ell^+ b_\ell b_\ell + 6K b_\ell - K \sum_{r'} b_{\ell+r'} , \qquad \text{(B3)}$$

or by Equation (B2)

$$[F_{\ell,1} b_\ell, H] = 6K F_{\ell,1} b_\ell + pU_0 F_{\ell,2} b_\ell - K \sum_{r'} F_{\ell,1} b_{\ell+r'} ;$$

and Equation (B1) is correct for $j = 1$.

We assume Equation (B1) correct for $j = n$, i.e.,

$$[F_{\ell,m}\, b_\ell, H] = \begin{Bmatrix} [6K + (m-1)\rho U_0]\, F_{\ell,m}\, b_\ell \;+\; \rho U_0\, F_{\ell,m+1}\, b_\ell \\ -mK \sum_{r=1} F_{\ell,m}\, b_{\ell+r} \;+ (m-1)K \sum_{r=1} b^+_{\ell+r}\, F_{\ell,m-1}\, b_\ell\, b_\ell \end{Bmatrix}, \tag{B4}$$

and use this to verify Equation (B1) for $j = n + 1$, thus demonstrating the validity of this equation for all $j \geq 1$. Now

$$\begin{aligned} [F_{\ell,m+1}\, b_\ell, H] &= [(b^+_\ell)^m\, (b_\ell)^{m+1}, H] \\ &= [b^+_\ell\, F_{\ell,m}\, b_\ell\, b_\ell, H] \\ &= b^+_\ell\, F_{\ell,m}\, b_\ell\, b_\ell\, H - H\, b^+_\ell\, F_{\ell,m}\, b_\ell\, b_\ell \\ &= \begin{Bmatrix} b^+_\ell F_{\ell,m}\, b_\ell\, H\, b_\ell + b^+_\ell\, F_{\ell,m}\, b_\ell\, [b_\ell, H] \\ -b^+_\ell\, H\, F_{\ell,m}\, b_\ell\, b_\ell + [b^+_\ell, H]\, F_{\ell,m}\, b_\ell\, b_\ell \end{Bmatrix}, \end{aligned}$$

or

$$[F_{\ell,m+1}\, b_\ell, H] = b^+_\ell\, [F_{\ell,m}\, b_\ell, H]\, b_\ell + b^+_\ell\, F_{\ell,m}\, b_\ell\, [b_\ell, H] + [b^+_\ell, H]\, F_{\ell,m}\, b_\ell\, b_\ell . \tag{B5}$$

Now

$$[b_\ell, H]^+ = [H^+, b^+_\ell] = -[b^+_\ell, H^+];$$

and since H is Hermitian ($H = H^+$), we have

$$[b^+_\ell, H] = -[b_\ell, H]^+ .$$

Substituting Equation (B3) gives

$$\begin{aligned} [b^+_\ell, H] &= -\left[\rho U_0\, b^+_\ell\, b_\ell\, b_\ell + 6K b_\ell - K \sum_{r=1} b_{\ell+r}\right]^+ \\ &= -\rho U_0\, b^+_\ell\, b^+_\ell\, b_\ell - 6K\, b^+_\ell + K \sum_{r=1} b^+_{\ell+r} . \end{aligned} \tag{B6}$$

Consider the terms on the right-hand side of Equation (B5). Substituting Equation (B4) into the first of these terms gives

$$b_\ell^+ [F_{\ell,m} b_\ell, H] b_\ell = \begin{Bmatrix} [6K + (m-1)\rho U_0] b_\ell^+ F_{\ell,m} b_\ell b_\ell & + \rho U_0 b_\ell^+ F_{\ell,m+1} b_\ell b_\ell \\ -mK \sum_{r'} b_\ell^+ F_{\ell,m} b_\ell b_{\ell+r'} & + (m-1) K \sum_{r'} b_{\ell+r'}^+ b_\ell^+ F_{\ell,m-1} b_\ell b_\ell b_\ell \end{Bmatrix} \tag{B7}$$

$$= \begin{Bmatrix} [6K + (m-1)\rho U_0] F_{\ell,m+1} b_\ell & + \rho U_0 F_{\ell,m+2} b_\ell \\ -mK \sum_{r'} F_{\ell,m+1} b_\ell & + (m-1) K \sum_{r'} b_{\ell+r'}^+ F_{\ell,m} b_\ell b_\ell \end{Bmatrix} .$$

Substituting Equations (B3) and (B6) into the second and third terms gives

$$b_\ell^+ F_{\ell,m} b_\ell [b_\ell, H] + [b_{\ell'}^+, H] F_{\ell,m} b_\ell b_\ell \tag{B8}$$

$$= \begin{Bmatrix} b_\ell^+ F_{\ell,m} b_\ell [\rho U_0 b_\ell^+ b_\ell b_\ell + 6K b_\ell - K \sum_{r'} b_{\ell+r'}] \\ + [-\rho U_0 b_\ell^+ b_\ell^+ b_\ell - 6K b_\ell^+ + K \sum_{r'} b_{\ell+r'}^+] F_{\ell,m} b_\ell b_\ell \end{Bmatrix}$$

$$= \begin{Bmatrix} \rho U_0 [b_\ell^+ F_{\ell,m} b_\ell b_\ell^+ b_\ell b_\ell - b_\ell^+ b_\ell^+ b_\ell F_{\ell,m} b_\ell b_\ell] \\ -K \sum_{r'} F_{\ell,m+1} b_{\ell+r'} + K \sum_{r'} b_{\ell+r'}^+ F_{\ell,m} b_\ell b_\ell \end{Bmatrix} .$$

But

$$b_\ell^+ F_{\ell,m} b_\ell b_\ell^+ b_\ell b_\ell - b_\ell^+ b_\ell^+ b_\ell F_{\ell,m} b_\ell b_\ell$$

$$= (b_\ell^+)^m (b_\ell)^m b_\ell^+ b_\ell b_\ell - b_\ell^+ b_\ell^+ b_\ell (b_\ell^+)^{m-1} (b_\ell)^{m+1}$$

$$= \begin{Bmatrix} (b_\ell^+)^{m+1} (b_\ell)^{m+2} + m (b_\ell^+)^m (b_\ell)^{m+1} \\ -(b_\ell^+)^{m+1} (b_\ell)^{m+2} - (m-1) (b_\ell^+)^m (b_\ell)^{m+1} \end{Bmatrix}$$

$$= (b_\ell^+)^m (b_\ell)^{m+1} = F_{\ell,m+1}\, b_\ell ,$$

and so Equation (B8) becomes

$$b_\ell^+ F_{\ell,m} b_\ell [b_\ell, H] + [b_\ell^+, H] F_{\ell,m} b_\ell b_\ell \tag{B9}$$

$$= pU_0 F_{\ell,m+1} b_\ell - K \sum_{r'} F_{\ell,m+1} b_{\ell+r'} + K \sum_{r'} b_{\ell+r'}^+ F_{\ell,m} b_\ell b_\ell$$

Substitution of Equations (B7) and (B9) into Equation (B5) gives

$$[F_{\ell,m+1} b_\ell, H] = \left\{ \begin{array}{l} [6K + (m-1)pU_0] F_{\ell,m+1} b_\ell + pU_0 F_{\ell,m+2} b_\ell \\ -mK \sum_{r'} F_{\ell,m+1} b_{\ell+r'} + (m-1)K \sum_{r'} b_{\ell+r'}^+ F_{\ell,m} b_\ell b_\ell \\ + pU_0 F_{\ell,m+1} b_\ell - K \sum_{r'} F_{\ell,m+1} b_{\ell+r'} + K \sum_{r'} b_{\ell+r'}^+ F_{\ell,m} b_\ell b_\ell \end{array} \right\}$$

$$= \left\{ \begin{array}{l} (6K + mpU_0) F_{\ell,m+1} b_\ell + pU_0 F_{\ell,m+2} b_\ell \\ -(m+1)K \sum_{r'} F_{\ell,m+1} b_{\ell+r'} + mK \sum_{r'} b_{\ell+r'}^+ F_{\ell,m} b_\ell b_\ell \end{array} \right\} ,$$

which is Equation (B1) for $j = n + 1$, completing the proof of this equation by induction.

APPENDIX C

EVALUATION OF $\gamma(x)$, $h(x)$, $\Delta(x)$, AND $\varepsilon(x)$ FOR SMALL x

The functions γ, h, Δ, and ε in Chapter VI by the following equations:

$$\frac{1}{\pi^3}\int_R \frac{3-xS}{\sqrt{1-6xS+x^2S^2+4\gamma(x)}}\,d^3\Theta = 3 \tag{C1}$$

$$h(x) = \frac{1}{\pi^3}\int_R S(3-xS)\,f(x,S)\,d^3\Theta \tag{C2}$$

$$\Delta(x) = \frac{1}{\pi^3}\int_R [1-xS+\gamma(x)]\,f(x,S)\,d^3\Theta - 1 \tag{C3}$$

$$\varepsilon(x) = 6K\left[1 - \frac{1}{6}h(x) + \frac{1}{6x}\Delta(x)\right], \tag{C4}$$

where

$$f(x,S) = \left[1-6xS+x^2S^2+4\gamma(x)\right]^{-1/2}, \tag{C5}$$

$$S = \sum_{i=1}^{3}\cos\Theta_i\,,$$

and R is the region $0 \le \theta_1, \theta_2, \theta_3 \le \pi$.

Recall that Equation (C1) defines $\gamma(x)$ for $0 \le x < x_0$. Once γ is determined Equations (C2), (C3), and (C4) allow a calculation of h, Δ, and ε. To obtain an expression for $\gamma(x)$ from Equation (C1) we expand $f(x,S)$ about $x = 0$ keeping terms to order x^2, i.e.,

$$f(x,S) = f_0 + f_0' x + \frac{1}{2} f_0'' x^2 \tag{C6}$$

where

$$f_0 = f(0, S)$$

$$f_0' = \left.\frac{\partial f(x,S)}{\partial x}\right|_{x=0}$$

$$f_0'' = \left.\frac{\partial^2 f(x,S)}{\partial x^2}\right|_{x=0} .$$

Differentiating Equation (C5) with respect to x gives

$$\frac{\partial f}{\partial x} = -\frac{1}{2}\left[1 - 6xS + x^2S^2 + 4\gamma\right]^{-3}\left[-6S + 2xS^2 + 4\gamma'\right]$$

$$= (3S - xS^2 - 2\gamma')f^3 .$$

A second differentiation gives

$$\frac{\partial^2 f}{\partial x^2} = -(S^2 + 2\gamma'')f^3 + 3(3S - xS^2 - 2\gamma')f^2\frac{\partial f}{\partial x}$$

$$= -(S^2 + 2\gamma'')f^3 + 3(3S - xS^2 - 2\gamma')^2 f^5 .$$

Thus

$$f_0 = [1 + 4\gamma_0]^{-1/2} \tag{C7}$$

$$f_0' = (3S - 2\gamma_0')f_0^3 \tag{C8}$$

$$f_0'' = -(S^2 + 2\gamma_0'')f_0^3 + 3(3S - 2\gamma_0')^2 f_0^5 , \tag{C9}$$

where

$$\gamma_0 = \gamma(0)$$

$$\gamma_0' = \left.\frac{d\gamma(x)}{dx}\right|_{x=0}$$

$$\gamma_0'' = \left.\frac{d^2\gamma(x)}{dx^2}\right|_{x=0} .$$

Substituting Equation (C6) into Equation (C1) we get

$$\frac{1}{\pi^3}\int_R (3-xS)\left(f_o + f_o' x + \tfrac{1}{2} f_o'' x^2\right)\, d^3\Theta = 3$$

or to order x^2

$$\frac{3}{\pi^3}\int_R f_o\, d^3\Theta + \left[\frac{1}{\pi^3}\int_R (3f_o' - f_o S)\, d^3\Theta\right] x + \left[\frac{1}{\pi^3}\int_R \left(\tfrac{3}{2} f_o'' - f_o' S\right) d^3\Theta\right] x^2 = 3.$$

Since the value of x may be varied without changing the coefficients of this equation, we conclude

$$\frac{1}{\pi^3}\int_R f_o\, d^3\Theta = 1 \tag{C10}$$

$$\frac{1}{\pi^3}\int_R (3f_o' - f_o S)\, d^3\Theta = 0 \tag{C11}$$

$$\frac{1}{\pi^3}\int_R \left(\tfrac{3}{2} f_o'' - f_o' S\right) d^3\Theta = 0 \,. \tag{C12}$$

Substituting Equation (C7) into Equation (C10) we get

$$\frac{1}{\pi^3}\int_R (1+4\gamma_o)^{-1/2}\, d^3\Theta = 1$$

or

$$(1+4\gamma_o)^{-1/2} = 1 \,;$$

which requires

$$\gamma_o = 1 \,, \tag{C13}$$

and so

$$f_o = 1 \,. \tag{C14}$$

Upon substituting Equations (C8) and (C14) into Equation (C11) we obtain

$$\frac{1}{\pi^3}\int \left[9S - 6\gamma_o' - S\right] d^3\Theta = 0 \,,$$

or

$$\gamma_0' = \frac{4}{3\pi^3}\int_R S\, d^3\Theta = \frac{4}{3\pi^3}\int_0^{\pi}\int_0^{\pi}\int_0^{\pi}(\cos\theta_1+\cos\theta_2+\cos\theta_3)\,d\theta_1\,d\theta_2\,d\theta_3 = 0, \quad \text{(C15)}$$

and so

$$f_0' = 3S. \quad \text{(C16)}$$

Combining Equations (C9), (C12), (C14), and (C15) gives

$$\frac{1}{\pi^3}\int_R \left[\frac{3}{2}(-S^2-2\gamma_0'+27S^2)-3S^2\right] d^3\Theta = 0,$$

or

$$\frac{1}{\pi^3}\int_R (36S^2-3\gamma_0'')\,d^3\Theta = 0,$$

or

$$\gamma_0'' = 12\left[\frac{1}{\pi^3}\int_R S^2\, d^3\Theta\right]. \quad \text{(C17)}$$

Now

$$S^2 = \left(\sum_{i=1}^{3}\cos\Theta_i\right)^2 \quad \text{(C18)}$$

$$= \sum_{i=1}^{3}\cos^2\Theta_i + 2\sum_{1=i<j}^{3}\cos\Theta_i\cos\Theta_j;$$

and therefore

$$\frac{1}{\pi^3}\int_R S^2 d^3\Theta = \sum_{i=1}^{3}\frac{1}{\pi^3}\int_0^{\pi}\int_0^{\pi}\int_0^{\pi}\cos^2\Theta_i\,d\theta_1 d\theta_2 d\theta_3 + 2\sum_{1=i<j}^{3}\frac{1}{\pi^3}\int_0^{\pi}\int_0^{\pi}\int_0^{\pi}\cos\Theta_i\cos\Theta_j\,d\theta_1 d\theta_2 d\theta_3 \quad \text{(C19)}$$

$$= \frac{3}{\pi}\int_0^{\pi}\cos^2\Theta\, d\Theta = \frac{3}{2}.$$

Hence

$$\gamma_0'' = 18, \quad \text{(C20)}$$

and

$$f_0'' = 26S^2 - 36. \quad \text{(C21)}$$

To order x^2 the expansion for f is

$$f(x,S) = 1 + Sx + (13S^2 - 18)x^2 , \tag{C22}$$

while the corresponding expression for γ to the same order is

$$\gamma(x) = 9x^2 . \tag{C23}$$

In order to evaluate $h(x)$ for small x we substitute the expansion for f into Equation (C2) to get

$$\begin{aligned} h(x) &= \tfrac{1}{\pi^3}\int_R (3 - xS)S\left[1 + Sx + (13S^2 - 18)x^2\right] d^3\Theta \\ &= \tfrac{1}{\pi^3}\int_R \left[3S + 8S^2x + (36S^3 - 54S)x^2\right] d^3\Theta \\ &= \tfrac{3}{\pi^3}\int_R S\, d^3\Theta + \left[\tfrac{8}{\pi^3}\int_R S^2 d^3\Theta\right]x + \left[\tfrac{18}{\pi^3}\int_R (2S^3 - 3S) d^3\Theta\right]x^2 . \end{aligned} \tag{C24}$$

Any integral of the form

$$\int_R S^{2m+1}\, d^3\Theta \qquad\qquad n = 0,1,2. \ldots$$

must vanish since each term in $\left(\sum_{i=1}^{3} \cos\Theta_i\right)^{2m+1}$ involves at least one cosine function to an odd power which integrates over $[0,\pi]$ to zero. Hence

$$\int_R S\, d^3\Theta = \int_R S^3 d^3\Theta = 0 ;$$

and by Equation (C19)

$$\tfrac{1}{\pi^3}\int_R S^2 d^3\Theta = \tfrac{3}{2} ,$$

so that to order x^2

$$h(x) = 12x . \tag{C25}$$

The function Δ is evaluated for small x by inserting Equations (C22) and (C23) into Equation (C3) to get

$$\Delta(x) = \frac{1}{\pi^3}\int_R [1-Sx-9x^2][1+Sx+(13S^2-18)x^2]\,d^3\Theta - 1$$

$$= \frac{1}{\pi^3}\int_R [1+2Sx+(10S^2-9)x^2]\,d^3\Theta - 1$$

$$= \left[\frac{2}{\pi^3}\int_R S\,d^3\Theta\right]x + \left[\frac{1}{\pi^3}\int_R (10S^2-9)\,d^3\Theta\right]x^2,$$

or

$$\Delta(x) = 6x^2. \tag{C26}$$

The ground state energy per particle for small x is then

$$\varepsilon(x) = 6K\left[1 - \frac{1}{6}h(x) + \frac{1}{6x}\Delta(x)\right] \tag{C27}$$

$$= 6K(1-x).$$

Equations (C21), (C23), (C25), (C26), and (C27) are the results quoted in Chapter VI. A continuation of the calculations begun here gives

$$\gamma(x) = 9x^2 + 236.25x^4$$

$$f(x,S) = 1 + 3Sx + (13S^2-18)x^2 + (63S^3-162S)x^3 + (321S^4-1188S^2+13.5)x^4$$

$$h(x) = 12x + 288x^3$$

$$\Delta(x) = 6x^2 + 175.5x^4$$

$$\varepsilon(x) = 6K(1 - x - 18.75x^3).$$

APPENDIX D

ESTIMATE OF x_o

The critical value of x which marks the transition from solid to liquid is determined from Equation (133), that is

$$\frac{1}{\pi^3}\int_R \frac{3-x_o S}{\sqrt{(3-S)(6-3x_o-x_o S)}}\, d^3\theta = 3\sqrt{x_o}\,. \tag{D1}$$

To demonstrate that such an x_o exists consider the function

$$J(x) = \frac{1}{\pi^3}\int_R \frac{3-xS}{\sqrt{(3-S)(6-3x-xS)}}\, d^3\theta - 3\sqrt{x}$$

on the interval $0 \le x \le 1$. In particular

$$J(0) = \frac{1}{\pi^3}\int_R \frac{3}{\sqrt{6(3-S)}}\, d^3\theta > 0$$

and

$$J(1) = \frac{1}{\pi^3}\int_R \frac{3-S}{\sqrt{(3-S)(3-S)}}\, d^3\theta - 3 = 1-3 = -2 < 0.$$

For $0 < x < 1$

$$\frac{dJ}{dx} = -\frac{9(1-x)}{\pi^3}\int_R \frac{d^3\theta}{\sqrt{x^3(6-3x-xS)^3(3-S)}} - \frac{3}{2\sqrt{x}} < 0\,,$$

so that J decreases monotonically on this interval. Since J is continuous on $0 \le x \le 1$, since $J(0) > 0$ and $J(1) < 0$, and since J decreases monotonically on $0 < x < 1$, we conclude that there exists one, and only one, value of x on $0 < x < 1$, say x_o, such that

$$J(x_o) = 0\,.$$

But this is precisely the condition required by Equation (D1) for the critical value of x.

We estimate x_o by using Equation (D1). For $x_o << 1$,

$$3\sqrt{x_o} \simeq \frac{1}{\pi^3}\int_R \frac{3}{\sqrt{6(3-S)}}\, d^3\Theta$$

or

$$\sqrt{18x_o} \simeq \frac{1}{\pi^3}\int_R \left[1-\frac{S}{3}\right]^{-1/2} d^3\Theta . \tag{D2}$$

For all interior points of R, $\left|\frac{S}{3}\right| < 1$ and we may expand the integrand with the binomial theorem to get

$$\left[1-\frac{S}{3}\right]^{-1/2} = 1 + \frac{1}{6}S + \frac{1}{24}S^2 + \frac{5}{216}S^3 + \frac{35}{10368}S^4 + \cdots . \tag{D3}$$

Substituting this expansion into Equation (D2) gives

$$\sqrt{18x_o} = \left\{ \begin{array}{l} \frac{1}{\pi^3}\int_R d^3\Theta + \frac{1}{6}\left[\frac{1}{\pi^3}\int_R S\, d^3\Theta\right] + \frac{1}{24}\left[\frac{1}{\pi^3}\int_R S^2 d^3\Theta\right] \\ \quad + \frac{5}{216}\left[\frac{1}{\pi^3}\int_R S^3 d^3\Theta\right] + \frac{35}{10368}\left[\frac{1}{\pi^3}\int_R S^4 d^3\Theta\right] \end{array} \right\} . \tag{D4}$$

From Appendix C

$$\int_R S\, d^3\Theta = \int_R S^3\, d^3\Theta = 0 ,$$

and

$$\frac{1}{\pi^3}\int_R S^2\, d^3\Theta = \frac{3}{2} .$$

Now

$$S^4 = \left(\sum_{i=1}^{3}\cos\theta_i\right)^4$$

$$= \sum_{i=1}^{3}\cos^4\theta_i + 6\sum_{i=i<j}^{3}\cos^2\theta_i\cos^2\theta_j + \left\{ \begin{array}{l} \text{terms with at least} \\ \text{one odd power cosine} \\ \text{factor} \end{array} \right\} ,$$

and so

$$\frac{1}{\pi^3}\int_R S^4 d^3\Theta = \frac{3}{\pi}\int_0^{\pi} \cos^4\theta\, d\theta + 18\left(\frac{1}{\pi}\int_0^{\pi}\cos^2\theta\, d\theta\right)^2 = 3\left(\frac{3}{8}\right) + 18\left(\frac{1}{2}\right)^2 = \frac{45}{8}$$

Therefore

$$\sqrt{18 X_0} \simeq 1 + \frac{1}{24}\left(\frac{3}{2}\right) + \frac{35}{10368}\left(\frac{45}{8}\right) \simeq 1.08$$

and

$$X_0 \simeq \frac{(1.08)^2}{18} = 0.065 .$$

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